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1.

Requester's Full Name: EE - 1000 Examiner #: 1000 Date: 1/2/83
 Art Unit: 1000 Phone Number 301: 1000 Serial Number: 1000
 Mail Box and Bldg/Room Location: _____ Results Format Preferred (circle): PAPER DISK E-MAIL

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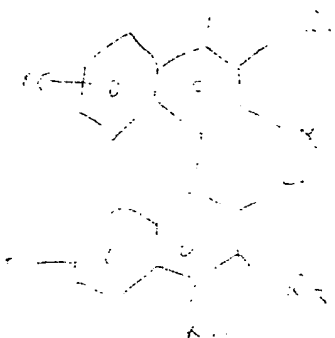
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names):

Earliest Priority Filing Date:

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*



Rob. Louch
Approved

77-14
SPE, A-10.

368-2927

van Soest
Reference Program
Biotechnology & Chemicals
CMA 197 - 1999-2000
Van Soest & Associates

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Searcher Location: _____

Date Searcher Picked Up: _____

Date Completed: _____

Searcher Prep & Review Time: _____

Clerical Prep Time: _____

Online Time: _____

Type of Search

NA Sequence (#)

AA Sequence (#)

Structure (#)

Bibliographic

Litigation

Fulltext

Patent Family

Other

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STN .

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Dr. Link

Lexis/Nexis

Sequence Systems

WWW/Internet

Other (specify) _____

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STRUCTURE FILE UPDATES: 11 MAY 2003 HIGHEST RN 514167-89-6
DICTIONARY FILE UPDATES: 11 MAY 2003 HIGHEST RN 514167-89-6

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

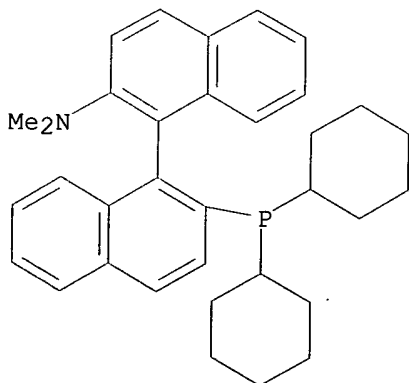
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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L11 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2003 ACS
RN 255882-16-7 REGISTRY
CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
(S)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (S)-(+)-2'-(Dicyclohexylphosphino)-N,N-dimethyl[1,1'-binaphthalen]-2-amine
MF C34 H40 N P
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1957 TO DATE)
4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 136:279128

REFERENCE 2: 135:107072

REFERENCE 3: 134:115733

REFERENCE 4: 132:108101

L11 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2003 ACS

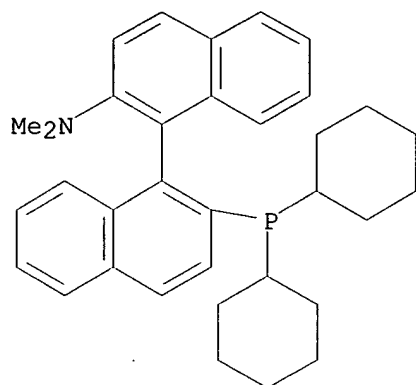
RN 255882-15-6 REGISTRY

CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
(R)- (9CI) (CA INDEX NAME)

MF C34 H40 N P

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1957 TO DATE)

4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:221639

REFERENCE 2: 136:309970

REFERENCE 3: 135:107072

REFERENCE 4: 132:108101

L11 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2003 ACS

RN 255835-81-5 REGISTRY

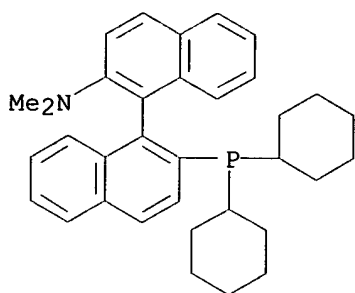
CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C34 H40 N P

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1957 TO DATE)
3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 135:318588

REFERENCE 2: 134:115733

REFERENCE 3: 132:108101

=> fil uspatall

FILE 'USPATFULL' ENTERED AT 08:52:53 ON 12 MAY 2003

CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 08:52:53 ON 12 MAY 2003

CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

=> d bib abs hitstr tot 118

L18 ANSWER 1 OF 3 USPATFULL
AN 2002:280844 USPATFULL
TI Ligands for metals and improved metal-catalyzed processes based thereon
IN Buchwald, Stephen L., Newton, MA, UNITED STATES
Old, David W., Somerville, MA, UNITED STATES
Wolfe, John P., Brighton, MA, UNITED STATES
Palucki, Michael, Belle Meade, NJ, UNITED STATES
Kamikawa, Ken, Brookline, MA, UNITED STATES
PI US 2002156295 A1 20021024
AI US 2001-4101 A1 20011023 (10)
RLI Continuation of Ser. No. US 1999-231315, filed on 13 Jan 1999, GRANTED,
Pat. No. US 6307087 Continuation-in-part of Ser. No. US 1998-113478,
filed on 10 Jul 1998, GRANTED, Pat. No. US 6395916
DT Utility
FS APPLICATION
LREP FOLEY HOAG LLP, PATENT GROUP, 155 SEAPORT BOULEVARD, BOSTON, MA, 02110
CLMN Number of Claims: 86
ECL Exemplary Claim: 1
DRWN 1 Drawing Page(s)
LN.CNT 4415
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB One aspect of the present invention relates to novel ligands for transition metals. A second aspect of the present invention relates to the use of catalysts comprising these ligands in transition metal-catalyzed carbon-heteroatom and carbon-carbon bond-forming reactions. The subject methods provide improvements in many features of the transition metal-catalyzed reactions, including the range of

suitable substrates, reaction conditions, and efficiency.

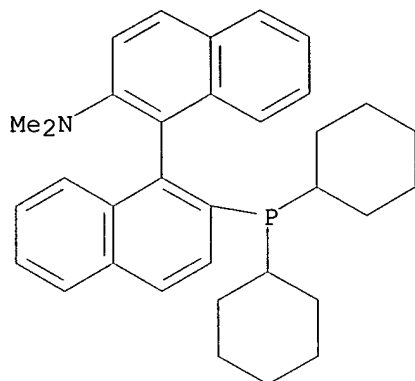
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 255882-15-6 255882-16-7

(catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

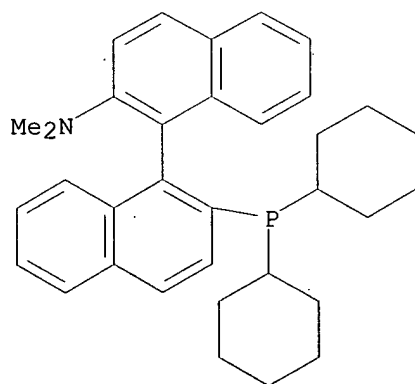
RN 255882-15-6 USPATFULL

CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-, (R)- (9CI) (CA INDEX NAME)



RN 255882-16-7 USPATFULL

CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-, (S)- (9CI) (CA INDEX NAME)

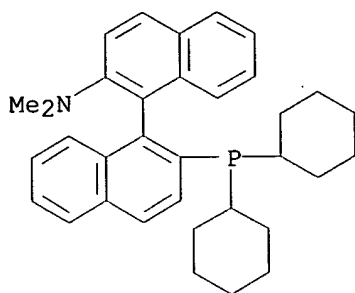


IT 255835-81-5P

(prepd. catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

RN 255835-81-5 USPATFULL

CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-, (9CI) (CA INDEX NAME)



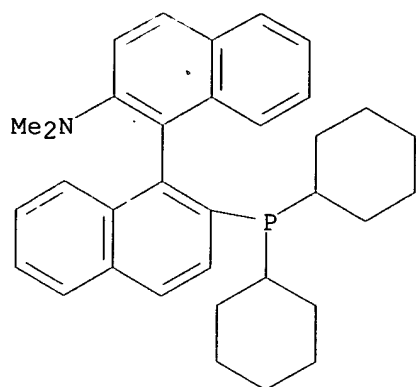
L18 ANSWER 2 OF 3 USPATFULL
 AN 2002:122783 USPATFULL
 TI Ligands for metals and improved metal-catalyzed processes based thereon
 IN Buchwald, Stephen L., Newton, MA, United States
 Wolfe, John P., Brighton, MA, United States
 Old, David W., Somerville, MA, United States
 Kamikawa, Ken, Brookline, MA, United States
 Palucki, Michael, Belle Meade, NJ, United States
 PA Massachusetts Institute of Technology, Cambridge, MA, United States
 (U.S. corporation)
 PI US 6395916 B1 20020528
 AI US 1998-113478 19980710 (9)
 DT Utility
 FS GRANTED
 EXNAM Primary Examiner: Higel, Floyd D.; Assistant Examiner: Sackey, Ebenezer
 LREP Gordon, Dana M., Foley, Hoag & Eliot LLP
 CLMN Number of Claims: 43
 ECL Exemplary Claim: 1
 DRWN 0 Drawing Figure(s); 0 Drawing Page(s)
 LN.CNT 4455

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

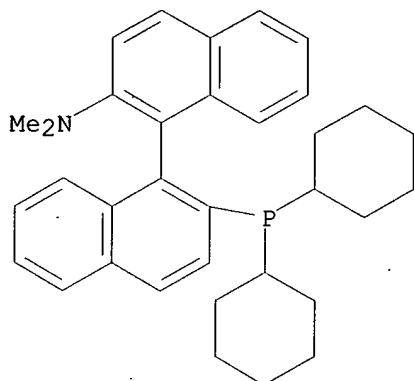
AB One aspect of the present invention relates to novel, electron-rich bidentate ligands for transition metals. A second aspect of the present invention relates to the use of catalysts comprising these ligands in transition metal-catalyzed carbon-heteroatom and carbon-carbon bond-forming reactions. The subject methods provide improvements in many features of the transition metal-catalyzed reactions, including the range of suitable substrates, reaction conditions, and efficiency.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 255882-15-6 255882-16-7
 (catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
 RN 255882-15-6 USPATFULL
 CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-, (R)- (9CI) (CA INDEX NAME)



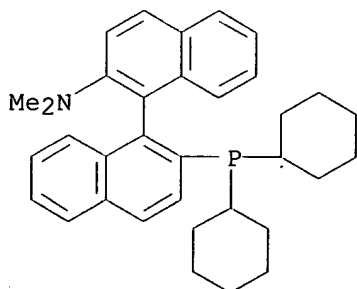
RN 255882-16-7 USPATFULL

CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
(S)- (9CI) (CA INDEX NAME)

IT 255835-81-5P

(prepd. catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

RN 255835-81-5 USPATFULL

CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
(9CI) (CA INDEX NAME)L18 ANSWER 3 OF 3 USPATFULL
AN 2001:185515 USPATFULL

TI Ligands for metals and improved metal-catalyzed processes based thereon
IN Buchwald, Stephen L., Newton, MA, United States
Old, David W., Somerville, MA, United States
Wolfe, John P., Brighton, MA, United States
Palucki, Michael, Belle Meade, NJ, United States
Kamikawa, Ken, Brookline, MA, United States
PA Massachusetts Institute of Technology, Cambridge, MA, United States
(U.S. corporation)
PI US 6307087 B1 20011023
AI US 1999-231315 19990113 (9)
RLI Continuation-in-part of Ser. No. US 1998-113478, filed on 10 Jul 1998
DT Utility
FS GRANTED
EXNAM Primary Examiner: Higel, Floyd D.; Assistant Examiner: Sackey, Ebenezer
LREP Gordon, Dana M.Foley Hoag & Eliot LLP
CLMN Number of Claims: 84
ECL Exemplary Claim: 1
DRWN 1 Drawing Figure(s); 1 Drawing Page(s)
LN.CNT 4650

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB One aspect of the present invention relates to novel ligands for transition metals. A second aspect of the present invention relates to the use of catalysts comprising these ligands in transition metal-catalyzed carbon-heteroatom and carbon-carbon bond-forming reactions. The subject methods provide improvements in many features of the transition metal-catalyzed reactions, including the range of suitable substrates, reaction conditions, and efficiency.

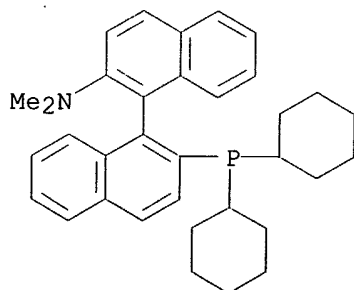
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT. 255835-81-5P

(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)

RN 255835-81-5 USPATFULL

CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-
(9CI) (CA INDEX NAME)



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FILE COVERS 1907 - 12 May 2003 VOL 138 ISS 20
FILE LAST UPDATED: 11 May 2003 (20030511/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L17 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2003 ACS
AN 2002:879182 HCAPLUS
DN 138:221639
TI Synthesis of aminophosphine ligands with binaphthyl backbones for silver(I)-catalyzed enantioselective allylation of benzaldehyde
AU Wang, Yi; Ji, Bao-Ming; Ding, Kui-Ling
CS State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SO Chinese Journal of Chemistry (2002), 20(11), 1300-1312
CODEN: CJOCEV; ISSN: 1001-604X
PB Science Press
DT Journal
LA English
CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 67
OS CASREACT 138:221639
AB Aminophosphine ligands with binaphthalene and octahydrobinaphthalene backbones were synthesized from 2-amino-2'-hydroxy-1,1'-binaphthyl (NOBIN) and 2-amino-2'-hydroxy-5,5',6,6',7,7',8,8'-octahydro-1,1'-binaphthyl (H8-NOBIN), resp. Asym. induction efficiency of silver(I)-ligand complexes was examd. for allylation of benzaldehyde with allyltributyltin, yielding 4-phenyl-4-hydroxy-1-butene (1). For example, (S)-1 was obtained (100% yield, 54.5% ee) under optimized reaction conditions via allylation catalyzed by silver(I)/(S)-(+)-2-pyrrolidino-2'-diphenylphosphino-1,1'-binaphthyl complex. Effects of binaphthyl backbone chirality and substituents at chelating N, P atoms on enantioselectivity are discussed.
ST aminophosphine binaphthyl octahydrobinaphthyl prepn allylation catalyst; benzaldehyde stereoselective allylation allyltin silver aminophosphinyl binaphthalene catalyzed
IT Allylation catalysts
Asymmetric synthesis and induction
(prepn. of aminophosphine ligands with binaphthalene and octahydrobinaphthalene backbones for silver-catalyzed enantioselective allylation of benzaldehyde with allyltributyltin)
IT Phosphines
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of aminophosphine ligands with binaphthalene and octahydrobinaphthalene backbones for silver-catalyzed enantioselective allylation of benzaldehyde with allyltributyltin)
IT Allylation
(stereoselective; prepn. of aminophosphine ligands with binaphthalene and octahydrobinaphthalene backbones for silver-catalyzed enantioselective allylation of benzaldehyde with allyltributyltin)
IT 2923-28-6 14104-20-2 26042-63-7 216368-93-3 328074-69-7
328074-70-0 328074-72-2 328074-73-3 328074-79-9
RL: CAT (Catalyst use); USES (Uses)

(prepn. of aminophosphine ligands with binaphthalene and octahydronaphthalene backbones for silver-catalyzed enantioselective allylation of benzaldehyde with allyltributyltin)

IT 255882-15-6P 413578-90-2P 413578-93-5P 413578-94-6P
413578-97-9P 413578-98-0P 500718-20-7P 500718-21-8P 500718-22-9P
500718-23-0P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. of aminophosphine ligands with binaphthalene and octahydronaphthalene backbones for silver-catalyzed enantioselective allylation of benzaldehyde with allyltributyltin)

IT 100-52-7, Benzaldehyde, reactions 110-52-1 2409-61-2 4559-70-0
6737-42-4 14717-29-4 24850-33-7 55933-41-0 145290-34-2
187344-92-9 216368-90-0 278800-79-6 311800-97-2 325797-63-5
326921-37-3 413578-87-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of aminophosphine ligands with binaphthalene and octahydronaphthalene backbones for silver-catalyzed enantioselective allylation of benzaldehyde with allyltributyltin)

IT 166276-11-5P 216368-92-2P 413578-86-6P 413578-89-9P 413578-91-3P
413578-92-4P 413578-95-7P 413578-96-8P 500718-24-1P 500718-25-2P
500718-26-3P 500718-27-4P 500718-28-5P 500718-30-9P 500718-31-0P
500718-32-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of aminophosphine ligands with binaphthalene and octahydronaphthalene backbones for silver-catalyzed enantioselective allylation of benzaldehyde with allyltributyltin)

IT 77118-87-7P 85551-57-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of aminophosphine ligands with binaphthalene and octahydronaphthalene backbones for silver-catalyzed enantioselective allylation of benzaldehyde with allyltributyltin)

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

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(34) Yanagisawa, A; Synlett 1997, P933 HCAPLUS

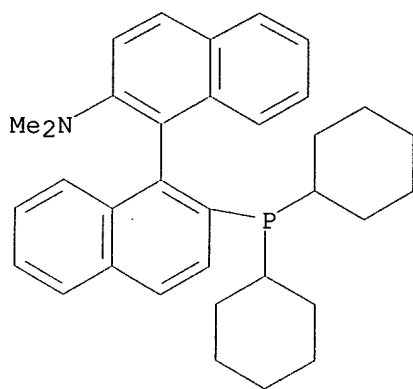
IT 255882-15-6P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)

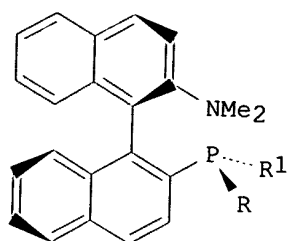
(prepn. of aminophosphine ligands with binaphthalene and
octahydronaphthalene backbones for silver-catalyzed enantioselective
allylation of benzaldehyde with allyltributyltin)

RN 255882-15-6 HCAPLUS

CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
(R)- (9CI) (CA INDEX NAME)



L17 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2003 ACS
AN 2002:116711 HCAPLUS
DN 136:309970
TI P-Chirogenic Binaphthyl-Substituted Monophosphines: Synthesis and Use in
Enolate Vinylation/Arylation Reactions
AU Hamada, Takayuki; **Buchwald, Stephen L.**
CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge,
MA, 02139, USA
SO Organic Letters (2002), 4(6), 999-1001
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 24, 75
OS CASREACT 136:309970
GI



I

- AB New phosphine ligands I (R = Ph, R1 = t-Bu; R = t-Bu, R1 = Ph) possessing both axial chirality and a chirogenic phosphorus center were prep'd. from (R)-2-bromo-2'-N,N-(dimethylamino)-1,1'-binaphthyl via a simple Li-halogen exchange protocol. The asym. vinylation of a ketone enolate with (R,RP)-2-(tert-butylphenylphosphino)-2'-N,N-(dimethylamino)-1,1'-binaphthyl I (R = Ph, R1 = t-Bu) afforded the coupling product with good enantiomeric excess.
- ST chirogenic binaphthyl phosphine prepn cocatalyst enolate vinylation arylation; crystal mol structure tert butylphenylphosphino dimethylamino binaphthyl; asym vinylation arylation ketone enolate palladium amino phosphino binaphthyl
- IT Crystal structure
Molecular structure
(of tert-butylphenylphosphino(dimethylamino)binaphthyl)
- IT Arylation catalysts
Asymmetric synthesis and induction
Vinylation catalysts
(prepn. of phosphorus-chirogenic binaphthyl-substituted monophosphines and their use in enolate vinylation/arylation reactions)
- IT 410083-22-6P
RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(crystal structure; prepn. of phosphorus-chirogenic binaphthyl-substituted monophosphines and their use in enolate vinylation/arylation reactions)
- IT 410071-71-5P 410084-17-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and phosphine deprotection of)
- IT 410083-24-8P 410083-25-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
- IT 350249-40-0P 405876-99-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 255882-15-6
RL: CAT (Catalyst use); USES (Uses)
(prepn. of phosphorus-chirogenic binaphthyl-substituted monophosphines and their use in enolate vinylation/arylation reactions)
- IT 410083-23-7P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of phosphorus-chirogenic binaphthyl-substituted monophosphines and their use in enolate vinylation/arylation reactions)
- IT 590-15-8 591-17-3 6057-79-0, tert-Butyl(phenyl)phosphine oxide
29949-69-7, tert-Butyl(chloro)phenylphosphine 350251-14-8 405877-16-9
RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of phosphorus-chirogenic binaphthyl-substituted monophosphines
and their use in enolate vinylation/arylation reactions)

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
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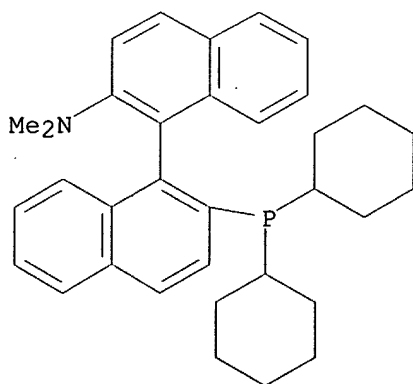
IT 255882-15-6

RL: CAT (Catalyst use); USES (Uses)

(prepn. of phosphorus-chirogenic binaphthyl-substituted monophosphines
and their use in enolate vinylation/arylation reactions)

RN 255882-15-6 HCAPLUS

CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
(R)- (9CI) (CA INDEX NAME)



L17 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2003 ACS

AN 2002:73750 HCAPLUS

DN 136:279128

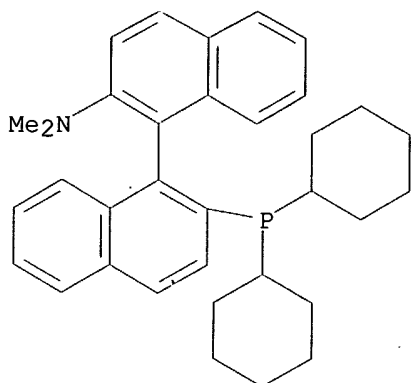
TI An Improved Catalyst for the Asymmetric Arylation of Ketone Enolates

AU Hamada, Takayuki; Chieffi, Andre; Ahman, Jens; Buchwald, Stephen
L.
CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge,
MA, 02139, USA
SO Journal of the American Chemical Society (2002), 124(7), 1261-1268
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
CC 24-4 (Alicyclic Compounds)
AB A new catalyst system for the enantioselective .alpha.-arylation of
ketones is reported. This catalyst, prepd. from Pd2(dba)3 and a bulky
dialkylphosphino-binaphthyl ligand, is able to effect the asym. arylation
of ketone enolates with aryl bromides utilizing NaOtBu as base. These new
catalysts enjoy much higher reactivity than previous systems; arylation
reactions could be effected at room temp. with only 2 mol % of the Pd
catalyst. The coupling of .alpha.-alkyl-.alpha.'-protected
cyclopentanones proceeded in high yield, and the resulting quaternary
stereogenic center was installed in up to 94% ee.
ST asym arylation enolate palladium dialkylphosphinobinaphthyl;
cyclopentanone enolate asym arylation palladium dialkylphosphinobinaphthyl
IT Enolates
RL: RCT (Reactant); RACT (Reactant or reagent)
(improved catalyst for asym. arylation of ketone enolates)
IT Arylation
Arylation catalysts
(stereoselective; improved catalyst for asym. arylation of ketone
enolates)
IT 3375-31-3, Palladium diacetate 51364-51-3 55700-44-2 76189-56-5,
(S)-BINAP 134484-36-9 139139-92-7 149341-34-4, (R)-QUINAP
255882-16-7 255882-18-9 350251-12-6 405877-62-5
RL: CAT (Catalyst use); USES (Uses)
(improved catalyst for asym. arylation of ketone enolates)
IT 405877-65-8P 405877-66-9P 405877-67-0P 405877-68-1P 405877-69-2P
405877-70-5P 405877-71-6P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)
(improved catalyst for asym. arylation of ketone enolates)
IT 95-46-5, o-Tolyl bromide 104-92-7, p-Bromoanisole 106-38-7, p-Tolyl
bromide 402-43-7 591-17-3, m-Tolyl bromide 1120-72-5,
2-Methylcyclopentanone 2398-37-0, m-Bromoanisole 3972-65-4
17789-14-9 53753-58-5, Diisopropylphosphine oxide 128544-05-8
405877-72-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(improved catalyst for asym. arylation of ketone enolates)
IT 405877-15-8P 405877-16-9P 405877-17-0P 405877-18-1P 405877-63-6P
405877-64-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(improved catalyst for asym. arylation of ketone enolates)
IT 22800-17-5P 405876-97-3P 405876-98-4P 405876-99-5P 405877-00-1P
405877-01-2P 405877-02-3P 405877-03-4P 405877-04-5P 405877-05-6P
405877-06-7P 405877-07-8P 405877-08-9P 405877-09-0P 405877-10-3P
405877-11-4P 405877-12-5P 405877-13-6P 405877-14-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(improved catalyst for asym. arylation of ketone enolates)
IT 100-61-8, N-Methylaniline, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with 2-formyl-5-methylcyclopentanone)
IT 109-94-4, Ethyl formate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with 2-methylcyclopentanone)
RE.CNT 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD

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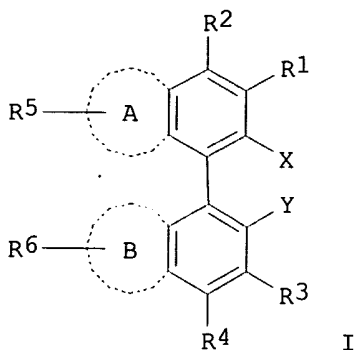
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 IT 255882-16-7
 RL: CAT (Catalyst use); USES (Uses)
 (improved catalyst for asym. arylation of ketone enolates)
 RN 255882-16-7 HCAPLUS
 CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
 (S)- (9CI) (CA INDEX NAME)



L17 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2003 ACS
 AN 2001:772171 HCAPLUS
 DN 135:318588
 TI Biaryl phosphine and amine ligands for improved transition metal-catalyzed processes
 IN Buchwald, Stephen L.; Old, David W.; Wolfe, John P.; Palucki, Michael; Kamikawa, Ken
 PA Massachusetts Institute of Technology, USA
 SO U.S., 55 pp., Cont.-in-part of U.S. Ser. No. 113,478.
 CODEN: USXXAM
 DT Patent
 LA English
 IC ICM C07C255-03
 ICS C07F009-28; C07D265-30; C07D211-70; C07D209-04
 NCL 558388000
 CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 25
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6307087	B1	20011023	US 1999-231315	19990113 <--
	US 6395916	B1	20020528	US 1998-113478	19980710 <--
	CA 2336691	AA	20000120	CA 1999-2336691	19990709 <--
	WO 2000002887	A2	20000120	WO 1999-US15450	19990709 <--
	WO 2000002887	A3	20000629		
	W: CA, JP				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1097158	A2	20010509	EP 1999-933785	19990709 <--	
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2002520328	T2	20020709	JP 2000-559117	19990709 <--
	US 2002156295	A1	20021024	US 2001-4101	20011023 <--
PRAI	US 1998-113478	A2	19980710		
	US 1998-196855	A	19981120		
	US 1999-231315	A	19990113		

US 1999-239024 A 19990127
 WO 1999-US15450 W 19990709 <--
 OS CASREACT 135:318588; MARPAT 135:318588
 GI



- AB The present invention relates to the prepn. of novel biaryl phosphine and amine ligands (I) [wherein A and B = independently fused monocyclic or polycyclic cycloalkyl, cycloalkenyl, aryl, or heterocyclic rings of 4-8 atoms; X = NR₂, PR₂, AsR₂, OR, or SR; Y = NR₂, PR₂, AsR₂, OR, SR, SiR₃, alkyl, or H; R-R₆ = independently H, halogen, (hetero)alkyl, alkenyl, alkynyl, hydroxy, alkoxy, silyloxy, amino, nitro, sulfhydryl, amide, carbonyl, ketone, anhydride, silyl, thioalkyl, ketone, ester, nitrile, (hetero)aryl, etc.] for transition metals and their use in metal-catalyzed carbon-heteroatom and carbon-carbon bond-forming reactions. Unexpected improvements over the prior art were demonstrated in transition metal-catalyzed aryl amination reactions, Suzuki couplings giving both biaryl and alkylaryl products, arylations and vinylations at the position .alpha. to carbonyl groups, and carbon-oxygen bond formation. The ligands and methods of the invention enable transformations utilizing aryl chlorides and bromides at room temp. at synthetically useful rates with extremely small amts. of catalyst relative to the limiting reagent. For example, coupling of p-chlorobenzonitrile and morpholine was catalyzed by 2.5 mol% Pd₂(dba)₃, 7.5 mol% of 2-(N,N-dimethylamino)-2'-(dicyclohexylphosphino)biphenyl, and NaOBu-t in DME at room temp. to provide 4-(4-morpholinyl)benzonitrile in 96% yield. Thus, the subject processes provide improvements in many features of the transition metal-catalyzed reactions, including the range of suitable substrates, reaction conditions, and efficiency.
- ST biaryl phosphine amine ligand prepn transition metal catalyst; amination aryl chloride bromide palladium catalysts; Suzuki coupling aryl chloride bromide palladium catalysts; ketone arylation palladium catalysts
- IT Amines, preparation
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (arom.; biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Ketones, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (arom.; biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Aryl halides
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (aryl chlorides; biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Chlorides, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)

- (aryl; biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Amination
Amination catalysts
Arylation
Arylation catalysts
Cross-coupling reaction catalysts
Suzuki coupling reaction
(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Phosphines
RL: CAT (Catalyst use); USES (Uses)
(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Biaryls
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Aryl bromides
RL: RCT (Reactant); RACT (Reactant or reagent)
(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Transition metal complexes
RL: CAT (Catalyst use); USES (Uses)
(phosphine; biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Phosphines
RL: CAT (Catalyst use); USES (Uses)
(transition metal complexes; biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT 127-09-3, Sodium acetate 534-17-8 584-08-7, Potassium carbonate 3375-31-3, Palladium diacetate 6476-37-5, Dicyclohexylphenylphosphine 7778-53-2 7789-23-3, Potassium fluoride 13400-13-0, Cesium fluoride 14221-01-3, Tetrakis(triphenylphosphine)palladium 51364-51-3, Tris(dibenzylideneacetone)dipalladium 54000-83-8, 2,6-Dimethoxyphenyl-di-t-butylphosphine 166330-10-5 213774-71-1 255837-14-0, 2,4,6-Trimethoxyphenyl-di-t-butylphosphine
RL: CAT (Catalyst use); USES (Uses)
(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT 213697-53-1P 224311-51-7P, 2-(Di-tert-butylphosphino)biphenyl 255835-81-5P 255835-82-6P
RL: CAT (Catalyst use); IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT 4688-76-0P 20837-12-1P 59734-92-8P 75295-57-7P 89291-23-6P 128796-39-4P, 4-(Trifluoromethyl)phenylboronic acid 157282-19-4P 213697-67-7P 224311-57-3P 224311-58-4P 224311-59-5P 255837-15-1P, 2-Bromo-4'(trifluoromethyl)biphenyl 255837-16-2P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT 92-69-3P, 4-Hydroxybiphenyl 92-91-1P, 4-Acetylbiphenyl 92-93-3P, 4-Nitrobiphenyl 612-75-9P, 3,3'-Dimethylbiphenyl 613-37-6P 644-08-6P 720-75-2P 825-55-8P, 2-Phenylthiophene 2142-66-7P, 2-Acetylbiphenyl 2920-38-9P, 4-Cyanobiphenyl 2928-43-0P, 2-Hydroxymethylbiphenyl 3976-34-9P, 2,6-Dimethylbiphenyl 4075-79-0P, n-Acetyl-4-aminobiphenyl 5405-15-2P 7372-85-2P, 2,5-Dimethylbiphenyl 10282-31-2P 17057-88-4P 19853-10-2P, [1,1'-Biphenyl]-2-acetonitrile 23676-05-3P 31144-33-9P 39253-43-5P 39910-98-0P, n-(4-Acetylphenyl)morpholine 54660-04-7P,

n-(4-Methoxyphenyl)pyrrolidine 76650-29-8P 76708-78-6P 81693-80-3P
82749-62-0P 92495-53-9P 138900-16-0P, N-(4-Fluorophenyl)indole
167283-32-1P, N-(4-Methylphenyl)indole 171092-38-9P,
3-(3-Acetylphenyl)pyridine 174307-96-1P 180336-54-3P,
N-(2,5-Dimethylphenyl)-N-methylaniline 197172-67-1P 213697-51-9P,
n-(2,5-Dimethylphenyl)morpholine 213697-52-0P 213697-65-5P
213697-66-6P 224311-54-0P 224311-55-1P 251320-77-1P 251320-78-2P
251320-81-7P, 3-Acetyl-3',5'-dimethoxybiphenyl 251320-82-8P,
4-Carbomethoxy-3'-acetylbiphenyl 251320-84-0P 255835-83-7P,
2(Di-t-butylphosphino)-4'-(trifluoromethyl)biphenyl 255835-84-8P
255835-85-9P 255882-14-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)

(biaryl phosphine and amine ligands for improved transition
metal-catalyzed processes)

IT 95-72-7 98-80-6 99-90-1 99-91-2 100-00-5, 1-Chloro-4-nitrobenzene
100-46-9, Benzylamine, reactions 100-61-8, n-Methylaniline, reactions
103-88-8, 4'-Bromoacetanilide 106-38-7 106-41-2, 4-Bromophenol
106-43-4 106-49-0, p-Toluidine, reactions 108-94-1, Cyclohexanone,
reactions 110-91-8, Morpholine, reactions 111-26-2, Hexylamine
111-92-2, Dibutylamine 120-72-9, Indole, reactions 123-75-1,
Pyrrolidine, reactions 402-43-7, 4-(Trifluoromethyl)phenyl bromide
460-00-4, 1-Bromo-4-fluorobenzene 553-94-6, 2-Bromo-p-xylene 556-96-7
563-80-4 565-69-5 576-22-7 583-53-9, 1,2-Dibromobenzene 583-55-1,
2-Bromiodobenzene 592-41-6, 1-Hexene, reactions 619-42-1 623-03-0,
4-Chlorobenzonitrile 623-12-1 626-60-8, 3-Chloropyridine 698-00-0
768-90-1, 1-Bromoadamantane 1003-09-4, 2-Bromothiophene 1013-88-3,
Benzophenone imine 1079-66-9, Chlorodiphenylphosphine 1122-91-4,
4-Bromobenzaldehyde 1126-46-1 2052-07-5, 2-Bromobiphenyl 2142-68-9,
2'-Chloroacetophenone 2856-63-5, 2-Chlorobenzyl cyanide 3972-65-4,
1-Bromo-4-t-butylbenzene 5720-06-9 7051-16-3 13716-10-4,
Chlorodi-tert-butylphosphine 16523-54-9, Chlorodicyclohexylphosphine
17933-03-8 18982-54-2, 2-Bromobenzylalcohol 22237-13-4,
4-Ethoxyphenylboronic acid 40138-16-7 42371-64-2 53847-33-9
74866-28-7, 2,2'-Dibromo-1,1'-binaphthyl 204841-19-0, 3-Acetylphenyl
boronic acid 251320-89-5, 2-(Bromo)-2'-(isopropyl)biphenyl

RL: RCT (Reactant); RACT (Reactant or reagent)

(biaryl phosphine and amine ligands for improved transition
metal-catalyzed processes)

RE.CNT 131 THERE ARE 131 CITED REFERENCES AVAILABLE FOR THIS RECORD
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- (9) Anon; 1995 HCAPLUS
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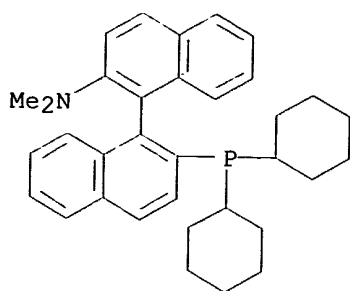
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IT 255835-81-5P

RL: CAT (Catalyst use); IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)

RN 255835-81-5 HCAPLUS

CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-
(9CI) (CA INDEX NAME)



- L17 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2003 ACS
 AN 2001:355541 HCAPLUS
 DN 135:107072
 TI Catalytic Asymmetric Vinylation of Ketone Enolates
 AU Chieffi, Andre; Kamikawa, Ken; Ahman, Jens; Fox, Joseph M.;
 Buchwald, Stephen L.
 CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge,
 MA, 02139, USA
 SO Organic Letters (2001), 3(12), 1897-1900
 CODEN: ORLEF7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 CC 24-1 (Alicyclic Compounds)
 OS CASREACT 135:107072
 AB A protocol for the catalytic asym. vinylation of ketone enolates has been
 developed. Key to the success of this process was the development of new
 electron-rich chiral monodentate ligands.
 ST asym vinylation ketone phosphine catalyst
 IT Asymmetric synthesis and induction
 Vinylation
 (catalytic asym. vinylation of ketone enolates)
 IT Vinylation catalysts
 (catalytic asym. vinylation of ketone enolates in presence of chiral
 phosphines)
 IT Ketones, preparation
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (cycloalkanones; catalytic asym. vinylation of ketone enolates)
 IT Vinyl compounds, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (halo; catalytic asym. vinylation of ketone enolates)
 IT 51364-51-3, Pd2(dba)3 213774-71-1
 RL: CAT (Catalyst use); USES (Uses)
 (catalytic asym. vinylation of ketone enolates)
 IT 233752-13-1P 255882-15-6P 255882-16-7P 255882-17-8P
 255882-18-9P 350251-12-6P
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
 USES (Uses)
 (catalytic asym. vinylation of ketone enolates)
 IT 350249-54-6P
 RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic
 preparation); PREP (Preparation); RACT (Reactant or reagent)
 (catalytic asym. vinylation of ketone enolates)
 IT 100-61-8, N-Methylaniline, reactions 103-63-9, 2-Bromoethylbenzene
 513-37-1 583-60-8, 2-Methylcyclohexanone 590-13-6,
 cis-1-Bromo-1-propene 590-15-8, trans-1-Bromo-1-propene 593-60-2,
 Bromoethene 1079-66-9, Chlorodiphenylphosphine 1120-72-5,

2-Methylcyclopentanone 1193-70-0, 2-Propylcyclopentanone 1590-08-5,
 2-Methyl-1-tetralone 3017-69-4 4819-67-4, 2-Pentylcyclopentanone
 16523-54-9, Chlorodicyclohexylphosphine 17496-14-9, 2-Methyl-1-indanone
 86688-06-4 224311-59-5 350249-56-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(catalytic asym. vinylation of ketone enolates)

IT 100717-47-3P 255837-20-8P 255837-21-9P 255837-22-0P 350249-40-0P
 350249-41-1P 350249-42-2P 350249-45-5P 350249-50-2P 350249-53-5P
 350249-55-7P 350251-13-7P 350251-14-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(catalytic asym. vinylation of ketone enolates)

IT 197163-99-8P 350249-43-3P 350249-44-4P 350249-46-6P 350249-47-7P
 350249-48-8P 350249-49-9P 350249-51-3P 350249-52-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(catalytic asym. vinylation of ketone enolates)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD

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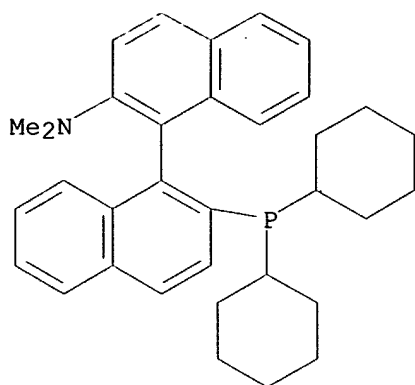
IT 255882-15-6P 255882-16-7P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
 USES (Uses)

(catalytic asym. vinylation of ketone enolates)

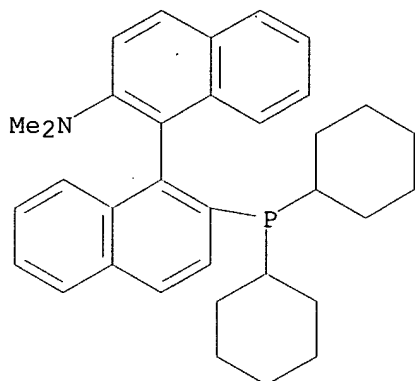
RN 255882-15-6 HCAPLUS

CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
 (R)- (9CI) (CA INDEX NAME)



RN 255882-16-7 HCAPLUS

CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
(S)- (9CI) (CA INDEX NAME)



L17 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2003 ACS

AN 2000:792828 HCAPLUS

DN 134:115733

TI A Catalytic Asymmetric Suzuki Coupling for the Synthesis of Axially Chiral Biaryl Compounds

AU Yin, Jingjun; Buchwald, Stephen L.

CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SO Journal of the American Chemical Society (2000), 122(48), 12051-12052
CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

CC 25-22 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

OS CASREACT 134:115733

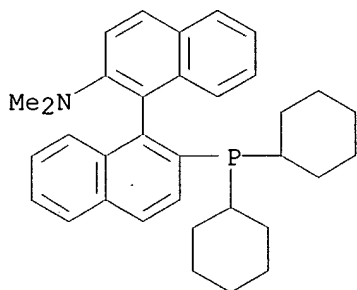
AB Binaphthyl ligands were used for the catalytic asym. Suzuki coupling to form highly enantiomerically enriched biaryl derivs. This is the first example of a catalytic enantioselective cross-coupling reaction that allows the prepn. of functionalized biaryl compds. For example, asym. Suzuki coupling of (1-bromo-2-naphthalenyl)phosphonic acid di-Me ester with (2-methylphenyl)boronic acid in the presence of (+)-(S)-2'-(dicyclohexylphosphino)-N,N-dimethyl-[1,1'-binaphthalen]-2-amine and Pd2(dba)3 gave (+)-[1-(2-methylphenyl)-2-naphthalenyl]phosphonic acid di-Me ester in 95% yield and in 86% enantiomeric excess. Subsequent

phenylation of the latter with phenylmagnesium bromide gave
 (-)-1-(2-methylphenyl)-2-(diphenylphosphinyl)naphthalene. Redn. of the
 latter gave (-)-[1-(2-methylphenyl)-2-naphthalenyl]diphenylphosphine.
 ST Suzuki coupling phosphinobinaphthalenamine palladium stereochem
 IT Coupling reaction catalysts
 (Suzuki; prepn. of axially chiral biaryl compds. via
 binaphthyl-catalyzed asym. Suzuki coupling)
 IT Stereochemistry
 Suzuki coupling reaction
 (prepn. of axially chiral biaryl compds. via binaphthyl-catalyzed asym.
 Suzuki coupling)
 IT Aryl halides
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of axially chiral biaryl compds. via binaphthyl-catalyzed asym.
 Suzuki coupling)
 IT 51364-51-3, Pd2(dba)3 98327-87-8 224311-52-8 **255835-81-5**
 255882-14-5 **255882-16-7**, (S)-(+)-2'-(Dicyclohexylphosphino)-N,N-
 dimethyl[1,1'-binaphthalen]-2-amine 320381-22-4 320381-23-5
 320767-12-2
 RL: CAT (Catalyst use); USES (Uses)
 (prepn. of axially chiral biaryl compds. via Suzuki coupling of
 arylboronic acids and halobenzene derivs. in presence of palladium and
 binaphthalene ligand)
 IT 88-73-3, 1-Chloro-2-nitrobenzene 577-19-5, 1-Bromo-2-nitrobenzene
 609-73-4, 1-Iodo-2-nitrobenzene 4688-76-0 16419-60-6,
 (2-Methylphenyl)boronic acid 89787-12-2, (2-Isopropylphenyl)boronic acid
 90002-36-1 320381-24-6 320381-25-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of axially chiral biaryl compds. via Suzuki coupling of
 arylboronic acids and halobenzene derivs. in presence of palladium and
 binaphthalene ligand)
 IT 100-58-3, Phenylmagnesium bromide 13922-41-3, (1-Naphthalenyl)boronic
 acid 219834-95-4 320381-26-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of axially chiral biaryl compds. via binaphthyl-catalyzed asym.
 Suzuki coupling)
 IT 320767-18-8P 320767-21-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. of axially chiral biaryl compds. via binaphthyl-catalyzed asym.
 Suzuki coupling)
 IT 132532-08-2P 320767-13-3P 320767-14-4P 320767-15-5P 320767-16-6P
 320767-17-7P 320767-19-9P 320767-20-2P 320767-22-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of axially chiral biaryl compds. via binaphthyl-catalyzed asym.
 Suzuki coupling)

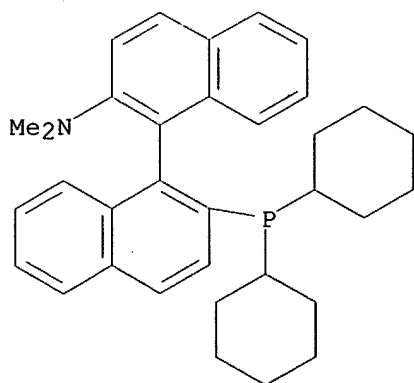
RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
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 IT 255835-81-5 255882-16-7, (S)-(+)-2'-
 (Dicyclohexylphosphino)-N,N-dimethyl[1,1'-binaphthalen]-2-amine
 RL: CAT (Catalyst use); USES (Uses)
 (prepn. of axially chiral biaryl compds. via Suzuki coupling of
 arylboronic acids and halobenzene derivs. in presence of palladium and
 binaphthalene ligand)
 RN 255835-81-5 HCAPLUS
 CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
 (9CI) (CA INDEX NAME)



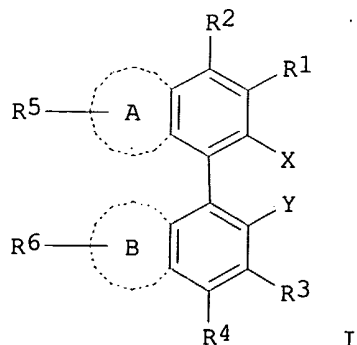
- RN 255882-16-7 HCAPLUS
 CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
 (S)- (9CI) (CA INDEX NAME)



AN 2000:53646 HCAPLUS
 DN 132:108101
 TI Biaryl phosphine and amine ligands for improved transition metal-catalyzed processes
 IN Buchwald, Stephen; Old, David W.; Wolfe, John P.; Palucki, Michael; Kamikawa, Ken; Chieffi, Andrew; Sadighi, Joseph P.; Singer, Robert A.; Ahman, Jens
 PA Massachusetts Institute of Technology, USA
 SO PCT Int. Appl., 397 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM C07F009-02
 CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 25

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 2000002887	A2	20000120	WO 1999-US15450	19990709 <--	
	WO 2000002887	A3	20000629			
	W: CA, JP					
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
	US 6395916	B1	20020528	US 1998-113478	19980710 <--	
	US 6307087	B1	20011023	US 1999-231315	19990113 <--	
	CA 2336691	AA	20000120	CA 1999-2336691	19990709 <--	
	EP 1097158	A2	20010509	EP 1999-933785	19990709 <--	
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
		JP 2002520328	T2	20020709	JP 2000-559117	19990709 <--
PRAI	US 1998-113478	A	19980710			
	US 1998-196855	A	19981120			
	US 1999-231315	A	19990113			
	US 1999-239024	A	19990127			
	WO 1999-US15450	W	19990709 <--			
OS	MARPAT 132:108101					
GI						



AB The present invention relates to the prepn. of novel biaryl phosphine and amine ligands (I) [wherein A and B = independently fused monocyclic or polycyclic cycloalkyl, cycloalkenyl, aryl, or heterocyclic rings of 4-8 atoms; X = NR₂, PR₂, AsR₂, OR, or SR; Y = NR₂, PR₂, AsR₂, OR, SR, SiR₃, alkyl, or H; R-R₆ = independently H, halogen, (hetero)alkyl, alkenyl, alkynyl, hydroxy, alkoxy, silyloxy, amino, nitro, sulfhydryl, amide,

carbonyl, ketone, anhydride, silyl, thioalkyl, ketone, ester, nitrile, (hetero)aryl, etc.] for transition metals and their use in metal-catalyzed carbon-heteroatom and carbon-carbon bond-forming reactions. Unexpected improvements over the prior art were demonstrated in transition metal-catalyzed aryl amination reactions, Suzuki couplings giving both biaryl and alkylaryl products, arylations and vinylations at the position .alpha. to carbonyl groups, and carbon-oxygen bond formation. The ligands and methods of the invention enable transformations utilizing aryl chlorides and bromides at room temp. at synthetically useful rates with extremely small amts. of catalyst relative to the limiting reagent. For example, coupling of p-chlorobenzonitrile and morpholine was catalyzed by 2.5 mol% Pd2(dba)3, 7.5 mol% of 2-(N,N-dimethylamino)-2'-(dicyclohexylphosphino)biphenyl, and NaOBu-t in DME at room temp. to provide 4-(4-morpholinyl)benzonitrile in 96% yield. Thus, the subject processes provide improvements in many features of the transition metal-catalyzed reactions, including the range of suitable substrates, reaction conditions, and efficiency.

ST biaryl phosphine ammine ligand prepn transition metal catalyst; amination aryl chloride bromide palladium catalysts; Suzuki coupling aryl chloride bromide palladium catalysts; ketone arylation vinylation palladium catalysts; etherification palladium catalysts .

IT Amines, preparation

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(arom.; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT Ethers, preparation

Ketones, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(arom.; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT Aryl halides

Aryl halides

RL: RCT (Reactant); RACT (Reactant or reagent)

(aryl chlorides; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT Chlorides, reactions

Chlorides, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(aryl; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT Transition metal complexes

Transition metal complexes

RL: CAT (Catalyst use); USES (Uses)

(phosphine; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT Amination

Amination catalysts

Arylation

Arylation catalysts

Cross-coupling reaction catalysts

Etherification

Etherification catalysts

Suzuki coupling reaction

Vinylation

Vinylation catalysts

(prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations,

- vinylations, and carbon-oxygen bond formation reactions)
- IT Phosphines
 RL: CAT (Catalyst use); USES (Uses)
 (prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Biaryls
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Aryl bromides
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Phosphines
 Phosphines
 RL: CAT (Catalyst use); USES (Uses)
 (transition metal complexes; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 534-17-8, Dicesium carbonate 3375-31-3, Diacetatopalladium 6476-37-5, Dicyclohexylphenylphosphine 14221-01-3, Tetrakis(triphenylphosphine)palladium 31570-04-4 51364-51-3, Tris(dibenzylideneacetone)dipalladium 54000-83-8, 2,6-Dimethoxyphenyl-di-t-butylphosphine 71042-54-1 74286-11-6 76189-56-5 91548-08-2 100165-88-6 133545-16-1 136779-28-7 139139-92-7 145964-33-6 149341-34-4 155806-35-2 213774-71-1 224311-49-3 247940-06-3 255837-14-0, 2,4,6-Trimethoxyphenyl-di-t-butylphosphine 255837-17-3 255837-19-5 255882-15-6 255882-16-7 255882-17-8 255882-18-9
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 698-00-0P 4688-76-0P 18937-92-3P 20837-12-1P, 2-Bromo-2'-methoxy-1,1'-biphenyl 59734-92-8P 75295-57-7P 89291-23-6P 89787-12-2P, 2-Isopropylphenylboronic acid 128796-39-4P, 4-(Trifluoromethyl)phenylboronic acid 224311-57-3P 224311-58-4P 224311-59-5P 251320-87-3P, 2-Bromo-2'-methylbiphenyl 251320-89-5P, 2-Bromo-2'-isopropylbiphenyl 255837-15-1P, 2-Bromo-4'-(trifluoromethyl)biphenyl 255837-16-2P 255837-18-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 213697-53-1P
 RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (prepd. catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 224311-51-7P, 2-(Di-tert-butylphosphino)biphenyl 224311-52-8P 224311-54-0P 224311-55-1P 251320-85-1P, 2-(Dicyclohexylphosphino)-2'-isopropylbiphenyl 251320-86-2P, 2-(Dicyclohexylphosphino)-2'-methylbiphenyl 255835-81-5P 255835-82-6P 255835-83-7P, 2-(Di-t-butylphosphino)-4'-(trifluoromethyl)biphenyl 255835-84-8P, 2-(Di-t-butylphosphino)-2'-(isopropyl)biphenyl 255835-85-9P 255836-32-9P 255836-65-8P 255836-67-0P 255836-68-1P, 1-[2-(Dicyclohexylphosphino)phenyl]naphthalene 255836-69-2P,

1-[2-(Di-t-butylphosphino)phenyl]naphthalene 255882-14-5P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)

(prepd. catalyst; prepn. of biaryl phosphine and amine ligands for
improved palladium-catalyzed amination reactions, Suzuki couplings,
arylations, vinylations, and carbon-oxygen bond formation reactions)

IT 62-53-3, Benzenamine, reactions 75-97-8 88-05-1 88-69-7 90-04-0
91-55-4 93-55-0, Propiophenone 95-65-8 95-68-1 95-72-7 96-22-0,
3-Pentanone 98-54-4 98-80-6 98-86-2, reactions 99-02-5 99-90-1
99-91-2 100-00-5, 1-Chloro-4-nitrobenzene 100-01-6, reactions
100-42-5, reactions 100-46-9, Benzenemethanamine, reactions 100-61-8,
reactions 103-69-5 103-88-8, 4'-Bromoacetanilide 104-92-7 104-94-9
105-53-3, Diethyl malonate 106-38-7 106-39-8 106-41-2, 4-Bromophenol
106-43-4 106-49-0, reactions 108-41-8 108-44-1, reactions
108-91-8, Cyclohexanamine, reactions 108-94-1, Cyclohexanone, reactions
109-01-3 109-04-6 109-09-1 110-89-4, Piperidine, reactions
110-91-8, Morpholine, reactions 111-26-2, 1-Hexanamine 111-92-2
119-61-9, Benzophenone, reactions 120-72-9, Indole, reactions 122-00-9
122-39-4, Diphenylamine, reactions 123-75-1, Pyrrolidine, reactions
141-97-9 280-64-8, 9-BBN 392-83-6, 2-Bromobenzotrifluoride 399-52-0
402-43-7, 4-(Trifluoromethyl)phenyl bromide 460-00-4,
1-Bromo-4-fluorobenzene 502-42-1, Cycloheptanone 504-02-9,
1,3-Cyclohexanedione 529-34-0 530-93-8, .beta.-Tetralone 540-88-5,
tert-Butyl acetate 553-94-6 556-96-7 557-93-7, 2-Bromopropene
563-80-4 565-69-5 565-80-0 576-22-7 576-26-1 583-53-9,
1,2-Dibromobenzene 583-55-1, 2-Bromiodobenzene 586-77-6 588-72-7,
trans-.beta.-Bromostyrene 590-15-8, trans-1-Bromopropene 591-20-8
592-41-6, 1-Hexene, reactions 615-36-1, 2-Bromoaniline 618-45-1
618-89-3 619-42-1 623-00-7, 4-Bromobenzonitrile 623-03-0 623-12-1
624-31-7 626-55-1, 3-Bromopyridine 626-60-8, 3-Chloropyridine
645-36-3 765-30-0, Cyclopropylamine 766-51-8 766-84-7 778-82-5
782-17-2 872-31-1, 3-Bromothiophene 873-32-5, 2-Chlorobenzonitrile
930-29-0, 1-Chlorocyclopentene 931-51-1, Cyclohexylmagnesium chloride
948-65-2 1003-09-4, 2-Bromothiophene 1013-88-3, Benzophenone imine
1079-66-9, Chlorodiphenylphosphine 1122-91-4, 4-Bromobenzaldehyde
1122-95-8 1126-46-1 1450-65-3 1590-08-5 2038-03-1,
4-Morpholineethanamine 2052-07-5, 2-Bromobiphenyl 2142-68-9,
2'-Chloroacetophenone 2398-37-0 2635-13-4 2845-89-8 2856-63-5,
2-Chlorobenzyl cyanide 2905-65-9 3972-65-4, 1-Bromo-4-t-butylbenzene
4079-52-1 4541-32-6 5350-57-2 5619-07-8, DL-Phenylalanine methyl
ester hydrochloride 5720-06-9 5798-75-4, Ethyl 4-bromobenzoate
5892-99-9 6781-98-2 7051-16-3 7073-94-1, 2-Bromoisopropylbenzene
7524-50-7, L-Phenylalanine methyl ester hydrochloride 7598-28-9
13716-10-4, Chlorodi-tert-butylphosphine 13922-41-3, 1-Naphthylboronic
acid 15499-27-1 16081-16-6 16419-60-6 16523-54-9,
Chlorodicyclohexylphosphine 17496-14-9, 2-Methylindanone 17763-70-1
17763-80-3 17789-14-9, 2-(3-Bromophenyl)1,3-dioxolane 17933-03-8
18982-54-2, 2-Bromobenzyl alcohol 22237-13-4, 4-Ethoxyphenylboronic acid
22867-74-9 24544-04-5 27505-78-8 27752-24-5 36800-95-0,
4-Cyanophenyl tosylate 40138-16-7, 2-Formylphenylboronic acid
41085-43-2, 2-Bromo-3-nitrotoluene 41492-05-1 42371-64-2 53847-33-9
66107-29-7 66107-32-2 74866-28-7, 2,2'-Dibromo-1,1'-binaphthyl
100379-00-8 100717-47-3 109613-00-5 112042-84-9 154318-75-9
157282-19-4 158266-43-4 204841-19-0, 3-Acetylphenylboronic acid
207611-58-3 255837-20-8 255837-21-9 255837-22-0 255837-23-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; prepn. of biaryl phosphine and amine ligands for
improved palladium-catalyzed amination reactions, Suzuki couplings,
arylations, vinylations, and carbon-oxygen bond formation reactions)

IT 78235-91-3P 213697-67-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(starting material; prepn. of biaryl phosphine and amine ligands for

- improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 251320-80-6P, N-(Diphenylmethylene)-2-bromoaniline
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthetic product; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 86-26-0P 92-69-3P, 4-Hydroxybiphenyl 92-91-1P, 4-Acetylbiphenyl 92-93-3P, 4-Nitrobiphenyl 101-70-2P, 4,4'-Dimethoxydiphenylamine 121-00-6P 613-37-6P, 4-Methoxybiphenyl 620-83-7P 620-93-9P, Di-p-tolylamine 644-08-6P, 4-Methylbiphenyl 720-75-2P, Methyl 4-phenylbenzoate 730-11-0P, 4-Methoxy-4'-nitrodiphenylamine 774-52-7P, N-(4-Methylphenyl)piperidine 825-54-7P 825-55-8P, 2-Phenylthiophene 1208-86-2P 1625-92-9P, 4-t-Butylbiphenyl 2142-66-7P, 2-Acetylbiphenyl 2920-38-9P, 4-Cyanobiphenyl 2928-43-0P, 2-(Hydroxymethyl)biphenyl 3077-16-5P, N-(4-Methylphenyl)morpholine 3470-65-3P 3976-34-9P, 2,6-Dimethylbiphenyl 4036-43-5P 4075-79-0P, N-Acetyl-4-aminobiphenyl 4316-51-2P, N-(4-Methoxyphenyl)-N,N-diphenylamine 4316-53-4P 4496-49-5P 4787-76-2P, N-(2-Methoxyphenyl)pyrrolidine 5031-78-7P 5405-15-2P, N-Benzyl-p-toluidine 5405-19-6P 6574-15-8P, N-(4-Nitrophenyl)piperidine 6935-27-9P, N-Benzyl-2-aminopyridine 7372-85-2P, 2,5-Dimethylbiphenyl 10273-87-7P 10282-31-2P, N-(4-Cyanophenyl)morpholine 15359-99-6P 15360-00-6P 16251-99-3P 16819-50-4P, N-(2,6-Dimethylphenyl)benzylamine 17057-88-4P, 3,5-Dimethylbiphenyl 17952-07-7P 19853-10-2P, [1,1'-Biphenyl]-2-acetonitrile 21218-94-0P 23600-89-7P 23676-05-3P 23699-65-2P, N-(3-Acetylphenyl)aniline 23951-29-3P 24255-25-2P, N-(2-Pyridyl)morpholine 25539-14-4P 25699-92-7P, N-(4-Cyanophenyl)indole 25700-23-6P, N-(3-Pyridyl)indole 27347-14-4P 31144-33-9P 31603-95-9P, 4-tert-Butyl-1-tert-butyloxybenzene 34160-16-2P 35393-20-5P, N-(Diphenylmethylene)-4-nitroaniline 38158-65-5P 38869-05-5P 39253-43-5P 39910-98-0P, N-(4-Acetylphenyl)morpholine 50798-94-2P, N-(2-Methoxyphenyl)benzylamine 50910-08-2P, N-(2-Pyridyl)-N,N-diphenylamine 51580-77-9P 51786-49-3P 52351-44-7P, N-(4-Methoxyphenyl)-2-phenylindole 54480-44-3P, 4-Methoxy-4'-(dimethylamino)diphenylamine 54660-04-7P, N-(4-Methoxyphenyl)pyrrolidine 55251-46-2P 56052-33-6P 56506-60-6P, N-(4-Methylphenyl)hexylamine 56915-80-1P, 1-(3-Acetylphenyl)-4-methylpiperazine 60893-66-5P 61394-81-8P 62787-14-8P 62787-15-9P 62790-83-4P 62790-85-6P 68856-26-8P 70945-85-6P 75201-55-7P 75934-30-4P 76650-29-8P, 4-Acetyl-3'-methylbiphenyl 76708-72-0P 76708-78-6P, 2,5,3'-Trimethylbiphenyl 77422-28-7P 81693-80-3P, 4-Hexylanisole 82749-62-0P 83188-35-6P 84736-47-0P, N-(4-t-Butylphenyl)morpholine 84736-54-9P, 2-(4-Methoxyphenyl)-3-pentanone 84839-92-9P 84839-93-0P 91949-95-0P, 4-Isopropoxybenzonitrile 92495-53-9P, 4-Methyl-2'-methoxybiphenyl 92670-29-6P, N-(3-Pyridyl)morpholine 93597-01-4P, N-(4-Methoxyphenyl)indole 94540-42-8P 94959-58-7P 97053-04-8P 97413-60-0P 114081-08-2P 114772-53-1P 116267-90-4P, N-(3-Thiophenyl)-N,N-diphenylamine 123324-87-8P 124043-95-4P 129644-26-4P 137445-01-3P 138900-16-0P, N-(4-Fluorophenyl)indole 138900-19-3P 146803-96-5P 167283-32-1P, N-(4-Methylphenyl)indole 171092-38-9P, 3-(3-Acetylphenyl)pyridine 172878-95-4P 174307-96-1P 175696-73-8P, N-(3-Cyanophenyl)pyrrolidine 179487-70-8P 180336-54-3P, N-(2,5-Dimethylphenyl)-N-methylaniline 183135-51-5P, N-Methyl-N-(3-pyridyl)aniline 183135-52-6P 185259-34-1P, N-(4-t-Butylphenyl)piperidine 188026-55-3P, N,N-Dibutyl-4-t-butylaniline 188026-64-4P, N-Ethyl-N-(3,5-dimethylphenyl)aniline 188026-74-6P 196604-19-0P 196604-21-4P 196604-24-7P 197172-67-1P 197172-69-3P 197640-99-6P 202802-70-8P 211292-60-3P 211292-66-9P, 2,6-Diisopropyl-2',6'-dimethyldiphenylamine 212382-74-6P 213014-13-2P 213697-51-9P 213697-52-0P, 2,6-Dimethyl-N-hexylaniline 213697-65-5P,

1,1-Bis(4-methylphenyl)-3-methyl-2-butanone 213697-66-6P 215394-88-0P
 223248-27-9P 223655-23-0P 224311-62-0P 224311-63-1P 224311-65-3P
 224311-66-4P 224311-67-5P 224311-68-6P 224311-69-7P 224311-70-0P
 224311-72-2P 224311-73-3P 224311-74-4P 224311-75-5P 224311-76-6P
 226569-78-4P 226917-75-5P, N-(4-Cyanophenyl)hexylamine 247940-07-4P,
 N-Methyl-N-(3,5-dimethoxyphenyl)aniline 247940-08-5P 251320-76-0P
 251320-77-1P, 4-Formyl-4'-ethoxybiphenyl 251320-78-2P 251320-79-3P
 251320-81-7P, 3-Acetyl-3',5'-dimethoxybiphenyl 251320-82-8P
 251320-83-9P 251320-84-0P, 2-Methoxy-2'-acetyl biphenyl 253768-96-6P,
 N-(3-Cyanophenyl)benzylamine 255835-86-0P 255835-87-1P 255835-88-2P
 255835-89-3P 255835-90-6P 255835-91-7P, N-(2,6-Dimethylphenyl)morpholine 255835-92-8P 255835-93-9P,
 N-(4-t-Butylphenyl)benzylamine 255835-94-0P, N-(3,4-Dimethylphenyl)pyrrolidine 255835-95-1P, 2-Methoxy-4'-cyanodiphenylamine 255835-96-2P 255835-97-3P 255835-98-4P 255835-99-5P 255836-00-1P
 255836-01-2P 255836-02-3P 255836-04-5P, N-(2-Methoxyphenyl)-N-(3-methoxyphenyl)-N-(4-methoxyphenyl)amine 255836-06-7P,
 N-(4-Dimethylaminophenyl)-N-(4-methoxyphenyl)-N-(3-methylphenyl)amine 255836-08-9P, N-(2,4-Dimethylphenyl)-N-(4-methoxyphenyl)-N-(3-methylphenyl)amine 255836-10-3P 255836-12-5P 255836-14-7P,
 N-(4-Butylphenyl)-N-(4-methoxyphenyl)-N-(4-methylphenyl)amine 255836-15-8P, N-(2,5-Dimethylphenyl)-N-(3,5-dimethylphenyl)-N-(4-methylphenyl)amine 255836-17-0P 255836-19-2P, N-(4-tert-Butylphenyl)indole 255836-21-6P 255836-23-8P, N-Cyclopropyl-4-tert-butylaniline 255836-25-0P, N-Cyclopropyl-2,5-dimethylaniline 255836-28-3P 255836-30-7P 255836-36-3P 255836-38-5P 255836-39-6P
 255836-41-0P 255836-43-2P 255836-44-3P 255836-45-4P, 2-Methyl-4-(4-butylphenyl)-3-pentanone 255836-46-5P 255836-48-7P
 255836-50-1P 255836-52-3P 255836-54-5P, 2-(3-Hydroxyphenyl)-3-pentanone 255836-56-7P, 2,4-Dimethyl-2-(4-t-butylphenyl)-3-pentanone 255836-57-8P 255836-59-0P 255836-61-4P 255836-63-6P 255836-70-5P,
 N-(4-t-Butylphenyl)-2-phenylindole 255836-72-7P 255836-74-9P, N-(3,5-Dimethylphenyl)-2,3-dimethylindole 255836-76-1P,
 N-(4-t-Butylphenyl)-2,3,7-trimethylindole 255836-78-3P 255836-80-7P, N-(2-Pyridyl)-7-ethylindole 255836-82-9P, N-(3,5-Dimethylphenyl)-7-ethylindole 255836-84-1P 255836-86-3P 255836-88-5P 255836-90-9P
 255836-92-1P 255836-94-3P 255836-95-4P 255836-96-5P 255836-97-6P
 255836-98-7P 255836-99-8P 255837-00-4P 255837-01-5P 255837-02-6P
 255837-03-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthetic product; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT 255837-04-8P 255837-05-9P 255837-06-0P 255837-07-1P 255837-08-2P
 255837-09-3P 255837-10-6P 255837-11-7P 255837-12-8P 255837-13-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthetic product; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

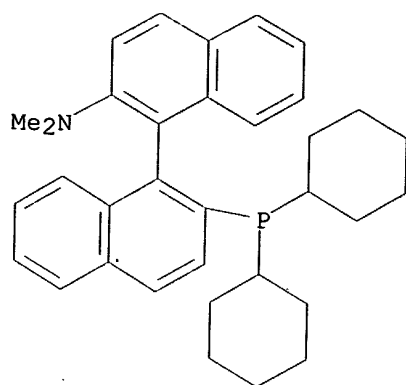
IT 255882-15-6 255882-16-7

RL: CAT (Catalyst use); USES (Uses)

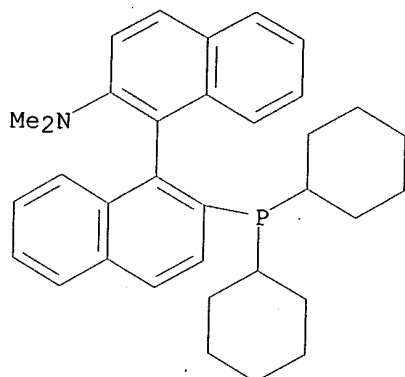
(catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

RN 255882-15-6 HCAPLUS

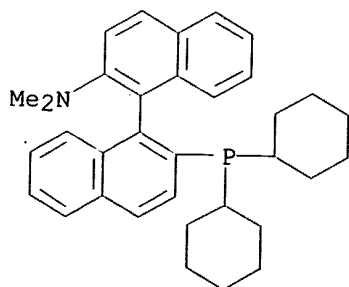
CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-, (R)- (9CI) (CA INDEX NAME)



RN 255882-16-7 HCAPLUS
 CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-,
 (S)- (9CI) (CA INDEX NAME)



IT 255835-81-5P
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
 USES (Uses)
 (prepd. catalyst; prepn. of biaryl phosphine and amine ligands for
 improved palladium-catalyzed amination reactions, Suzuki couplings,
 arylations, vinylations, and carbon-oxygen bond formation reactions)
 RN 255835-81-5 HCAPLUS
 CN [1,1'-Binaphthalen]-2-amine, 2'-(dicyclohexylphosphino)-N,N-dimethyl-
 (9CI) (CA INDEX NAME)



=> fil reg

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DICTIONARY FILE UPDATES: 11 MAY 2003 HIGHEST RN 514167-89-6

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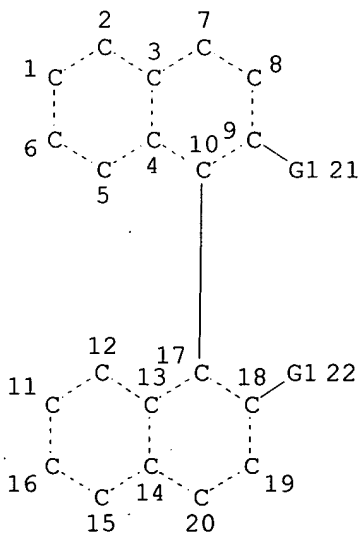
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Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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L19 STR



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VAR G1=N/P/AS/O/S

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L21 6721 SEA FILE=REGISTRY SSS FUL L19

100.0% PROCESSED 12141 ITERATIONS

SEARCH TIME: 00.00.01

6721 ANSWERS

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(FILE 'REGISTRY' ENTERED AT 08:54:49 ON 12 MAY 2003)
L21 6721 S L19 FUL

SAV TEMP L21 SACKY004/A

L22 6718 S L21 NOT L11

L23 7 S L22 AND L10

L24 5728 S L22 NOT (PMS OR CCS OR MNS)/CI

FILE 'HCAPLUS' ENTERED AT 08:59:36 ON 12 MAY 2003
L25 4102 S L22

L26 44 S L1-L9 AND L25
SEL HIT RN

FILE 'REGISTRY' ENTERED AT 09:00:08 ON 12 MAY 2003
L27 50 S E490-E539

FILE 'HCAPLUS' ENTERED AT 09:01:02 ON 12 MAY 2003
L28 2247 S L27
L29 44 S L26 AND L28
L30 22 S L29 AND (PY<=1998 OR PRY<=1998 OR AY<=1998)
L31 7 S L30 AND ORGANOMETAL?/SC,SX
L32 35 S L27 (L) CAT/RL AND L29
L33 15 S L30 AND L32
L34 19 S L31,L33

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L34 ANSWER 1 OF 19 HCAPLUS COPYRIGHT 2003 ACS
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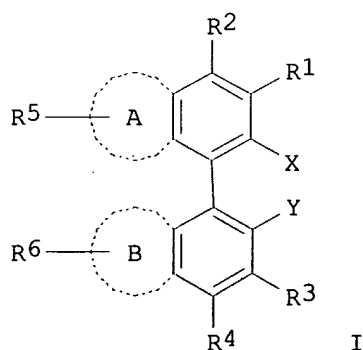
DN 135:318588

TI Biaryl phosphine and amine ligands for improved transition metal-catalyzed processes

IN Buchwald, Stephen L.; Old, David W.; Wolfe, John
P.; Palucki, Michael; Kamikawa, Ken

PA Massachusetts Institute of Technology, USA
 SO U.S., 55 pp., Cont.-in-part of U.S. Ser. No. 113,478.
 CODEN: USXXAM
 DT Patent
 LA English
 IC ICM C07C255-03
 ICS C07F009-28; C07D265-30; C07D211-70; C07D209-04
 NCL 558388000
 CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 25
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6307087	B1	20011023	US 1999-231315	19990113 <--
	US 6395916	B1	20020528	US 1998-113478	19980710 <--
	CA 2336691	AA	20000120	CA 1999-2336691	19990709 <--
	WO 2000002887	A2	20000120	WO 1999-US15450	19990709 <--
	WO 2000002887	A3	20000629		
	W: CA, JP				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	EP 1097158	A2	20010509	EP 1999-933785	19990709 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2002520328	T2	20020709	JP 2000-559117	19990709 <--
	US 2002156295	A1	20021024	US 2001-4101	20011023 <--
PRAI	US 1998-113478	A2	19980710	<--	
	US 1998-196855	A	19981120	<--	
	US 1999-231315	A	19990113		
	US 1999-239024	A	19990127		
	WO 1999-US15450	W	19990709	<--	
OS	CASREACT 135:318588; MARPAT 135:318588				
GI					



AB The present invention relates to the prepn. of novel biaryl phosphine and amine ligands (I) [wherein A and B = independently fused monocyclic or polycyclic cycloalkyl, cycloalkenyl, aryl, or heterocyclic rings of 4-8 atoms; X = NR₂, PR₂, AsR₂, OR, or SR; Y = NR₂, PR₂, AsR₂, OR, SR, SiR₃, alkyl, or H; R-R₆ = independently H, halogen, (hetero)alkyl, alkenyl, alkynyl, hydroxy, alkoxy, silyloxy, amino, nitro, sulfhydryl, amide, carbonyl, ketone, anhydride, silyl, thioalkyl, ketone, ester, nitrile, (hetero)aryl, etc.] for transition metals and their use in metal-catalyzed carbon-heteroatom and carbon-carbon bond-forming reactions. Unexpected improvements over the prior art were demonstrated in transition metal-catalyzed aryl amination reactions, Suzuki couplings giving both biaryl and alkylaryl products, arylations and vinylations at the position

.alpha. to carbonyl groups, and carbon-oxygen bond formation. The ligands and methods of the invention enable transformations utilizing aryl chlorides and bromides at room temp. at synthetically useful rates with extremely small amts. of catalyst relative to the limiting reagent. For example, coupling of p-chlorobenzonitrile and morpholine was catalyzed by 2.5 mol% Pd2(dba)3, 7.5 mol% of 2-(N,N-dimethylamino)-2'-(dicyclohexylphosphino)biphenyl, and NaOBu-t in DME at room temp. to provide 4-(4-morpholinyl)benzonitrile in 96% yield. Thus, the subject processes provide improvements in many features of the transition metal-catalyzed reactions, including the range of suitable substrates, reaction conditions, and efficiency.

- ST biaryl phosphine amine ligand prepn transition metal catalyst; amination aryl chloride bromide palladium catalysts; Suzuki coupling aryl chloride bromide palladium catalysts; ketone arylation palladium catalysts
- IT Amines, preparation
 - RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 - (arom.; biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Ketones, preparation
 - RL: SPN (Synthetic preparation); PREP (Preparation)
 - (arom.; biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Aryl halides
 - RL: RCT (Reactant); RACT (Reactant or reagent)
 - (aryl chlorides; biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Chlorides, reactions
 - RL: RCT (Reactant); RACT (Reactant or reagent)
 - (aryl; biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Amination
 - Amination catalysts
 - Arylation
 - Arylation catalysts
 - Cross-coupling reaction catalysts
 - Suzuki coupling reaction
 - (biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Phosphines
 - RL: CAT (Catalyst use); USES (Uses)
 - (biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Biaryls
 - RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 - (biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Aryl bromides
 - RL: RCT (Reactant); RACT (Reactant or reagent)
 - (biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Transition metal complexes
 - RL: CAT (Catalyst use); USES (Uses)
 - (phosphine; biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT Phosphines
 - RL: CAT (Catalyst use); USES (Uses)
 - (transition metal complexes; biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)
- IT 127-09-3, Sodium acetate 534-17-8 584-08-7, Potassium carbonate
 3375-31-3, Palladium diacetate 6476-37-5, Dicyclohexylphenylphosphine
 7778-53-2 7789-23-3, Potassium fluoride 13400-13-0, Cesium fluoride

14221-01-3, Tetrakis(triphenylphosphine)palladium 51364-51-3,
Tris(dibenzylideneacetone)dipalladium 54000-83-8, 2,6-Dimethoxyphenyl-di-
t-butylphosphine 166330-10-5 **213774-71-1** 255837-14-0,
2,4,6-Trimethoxyphenyl-di-t-butylphosphine

RL: CAT (Catalyst use); USES (Uses)

(biaryl phosphine and amine ligands for improved transition
metal-catalyzed processes)

IT 213697-53-1P 224311-51-7P, 2-(Di-tert-butylphosphino)biphenyl
255835-81-5P 255835-82-6P

RL: CAT (Catalyst use); IMF (Industrial manufacture); SPN (Synthetic
preparation); PREP (Preparation); USES (Uses)

(biaryl phosphine and amine ligands for improved transition
metal-catalyzed processes)

IT 4688-76-0P 20837-12-1P 59734-92-8P 75295-57-7P 89291-23-6P
128796-39-4P, 4-(Trifluoromethyl)phenylboronic acid 157282-19-4P
213697-67-7P 224311-57-3P 224311-58-4P 224311-59-5P 255837-15-1P,
2-Bromo-4'-(trifluoromethyl)biphenyl 255837-16-2P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent)

(biaryl phosphine and amine ligands for improved transition
metal-catalyzed processes)

IT 92-69-3P, 4-Hydroxybiphenyl 92-91-1P, 4-Acetylbiphenyl 92-93-3P,
4-Nitrobiphenyl 612-75-9P, 3,3'-Dimethylbiphenyl 613-37-6P 644-08-6P
720-75-2P 825-55-8P, 2-Phenylthiophene 2142-66-7P, 2-Acetylbiphenyl
2920-38-9P, 4-Cyanobiphenyl 2928-43-0P, 2-Hydroxymethylbiphenyl
3976-34-9P, 2,6-Dimethylbiphenyl 4075-79-0P, n-Acetyl-4-aminobiphenyl
5405-15-2P 7372-85-2P, 2,5-Dimethylbiphenyl 10282-31-2P 17057-88-4P
19853-10-2P, [1,1'-Biphenyl]-2-acetonitrile 23676-05-3P 31144-33-9P
39253-43-5P 39910-98-0P, n-(4-Acetylphenyl)morpholine 54660-04-7P,
n-(4-Methoxyphenyl)pyrrolidine 76650-29-8P 76708-78-6P 81693-80-3P
82749-62-0P 92495-53-9P 138900-16-0P, N-(4-Fluorophenyl)indole
167283-32-1P, N-(4-Methylphenyl)indole 171092-38-9P,
3-(3-Acetylphenyl)pyridine 174307-96-1P 180336-54-3P,
N-(2,5-Dimethylphenyl)-N-methylaniline 197172-67-1P 213697-51-9P,
n-(2,5-Dimethylphenyl)morpholine 213697-52-0P 213697-65-5P
213697-66-6P 224311-54-0P 224311-55-1P 251320-77-1P 251320-78-2P
251320-81-7P, 3-Acetyl-3',5'-dimethoxybiphenyl 251320-82-8P,
4-Carbomethoxy-3'-acetylbiphenyl 251320-84-0P 255835-83-7P,
2-(Di-tert-butylphosphino)-4'-(trifluoromethyl)biphenyl 255835-84-8P
255835-85-9P **255882-14-5P**

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)

(biaryl phosphine and amine ligands for improved transition
metal-catalyzed processes)

IT 95-72-7 98-80-6 99-90-1 99-91-2 100-00-5, 1-Chloro-4-nitrobenzene
100-46-9, Benzylamine, reactions 100-61-8, n-Methylaniline, reactions
103-88-8, 4'-Bromoacetanilide 106-38-7 106-41-2, 4-Bromophenol
106-43-4 106-49-0, p-Toluidine, reactions 108-94-1, Cyclohexanone,
reactions 110-91-8, Morpholine, reactions 111-26-2, Hexylamine
111-92-2, Dibutylamine 120-72-9, Indole, reactions 123-75-1,
Pyrrolidine, reactions 402-43-7, 4-(Trifluoromethyl)phenyl bromide
460-00-4, 1-Bromo-4-fluorobenzene 553-94-6, 2-Bromo-p-xylene 556-96-7
563-80-4 565-69-5 576-22-7 583-53-9, 1,2-Dibromobenzene 583-55-1,
2-Bromiodobenzene 592-41-6, 1-Hexene, reactions 619-42-1 623-03-0,
4-Chlorobenzonitrile 623-12-1 626-60-8, 3-Chloropyridine 698-00-0
768-90-1, 1-Bromoadamantane 1003-09-4, 2-Bromothiophene 1013-88-3,
Benzophenone imine 1079-66-9, Chlorodiphenylphosphine 1122-91-4,
4-Bromobenzaldehyde 1126-46-1 2052-07-5, 2-Bromobiphenyl 2142-68-9,
2'-Chloroacetophenone 2856-63-5, 2-Chlorobenzyl cyanide 3972-65-4,
1-Bromo-4-tert-butylbenzene 5720-06-9 7051-16-3 13716-10-4,
Chlorodi-tert-butylphosphine 16523-54-9, Chlorodicyclohexylphosphine
17933-03-8 18982-54-2, 2-Bromobenzylalcohol 22237-13-4,
4-Ethoxyphenylboronic acid 40138-16-7 42371-64-2 53847-33-9

74866-28-7, 2,2'-Dibromo-1,1'-binaphthyl 204841-19-0, 3-Acetylphenyl
boronic acid 251320-89-5, 2-(Bromo)-2'-(isopropyl)biphenyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(biaryl phosphine and amine ligands for improved transition
metal-catalyzed processes)

RE.CNT 131 THERE ARE 131 CITED REFERENCES AVAILABLE FOR THIS RECORD
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 (131) Zhao; Tetrahedron Letters 1996, V37(26), P4463 HCAPLUS

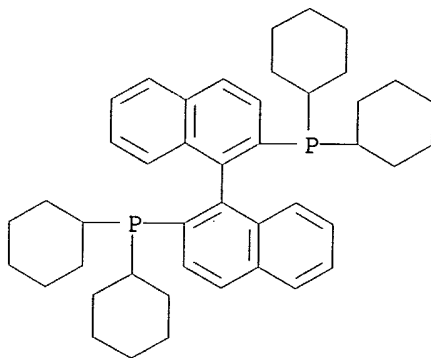
IT 213774-71-1

RL: CAT (Catalyst use); USES (Uses)

(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)

RN 213774-71-1 HCAPLUS

CN Phosphine, [1,1'-binaphthalene]-2,2'-diylbis[dicyclohexyl- (9CI) (CA INDEX NAME)



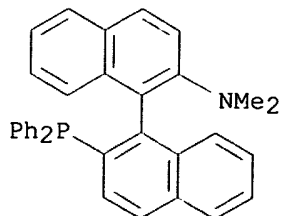
IT 255882-14-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)

RN 255882-14-5 HCAPLUS

CN [1,1'-Binaphthalen]-2-amine, 2'-(diphenylphosphino)-N,N-dimethyl- (9CI) (CA INDEX NAME)



DN 132:107774
 TI Transition metal catalyzed amination of aryl halides and triflates using imines.
 IN Wolfe, John P.; Ahman, Jens; Sadighi, Joseph P.; Singer, Robert A.; Buchwald, Stephen L.
 PA Massachusetts Institute of Technology, USA
 SO PCT Int. Appl., 61 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM C07C249-02
 ICS C07C251-04
 CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 27, 67
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000005199	A1	20000203	WO 1999-US16257	19990723 <--
	W: CA, JP				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 6323366	B1	20011127	US 1998-122324	19980724 <--
	CA 2336976	AA	20000203	CA 1999-2336976	19990723 <--
	EP 1100774	A1	20010523	EP 1999-937293	19990723 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2002521359	T2	20020716	JP 2000-561156	19990723 <--
PRAI	US 1998-122324	A	19980724	<--	
	US 1997-54092P	P	19970729	<--	
	WO 1999-US16257	W	19990723		
OS	CASREACT 132:107774; MARPAT 132:107774				
AB	ArN:CR1R2 [Ar = (substituted) (hetero)aryl; R1, R2 = H, (substituted) alkyl, alkenyl, alkynyl, (hetero)aryl, (hetero)arylalkyl, etc.; R1R2 = atoms to form a (substituted) ring], were prepd. by reaction of ArX (X = Cl, Br, iodo, OSO2X1, OSO2A, OSO2Ar; A = alkyl, X1 = halo) with RN:CR1R2 [R = H, trialkylstannyl, triarylstannyl, trialkylsilyl, triarylsilyl, Li, Na, K, Mg halide, Ca halide, Zn halide, B(OH)2, groups replaced by H under the reaction conditions] in the presence of a transition metal catalyst selected from groups 5-12 (Ni excepted) of the periodic table and a base selected from alkoxides, aryloxides, carbonates, amides, phosphates, and fluorides. Thus, Pd(OAc)2, bis(2-diphenylphosphino)phenyl ether, benzophenone imine, and 4-BrC6H4CMe3 were stirred in PhMe; NaOCMe3 was added and the mixt. was heated to 80.degree. to give 90% N-diphenylmethylen-4-tert-butylaniline.				
ST	aryl halide triflate imination transition metal catalyst imine; imine arom prepn				
IT	Amines, preparation				
	RL: SPN (Synthetic preparation); PREP (Preparation) (arom.; transition metal catalyzed amination of aryl halides and triflates using imines)				
IT	Imination				
	Imination (catalysts; transition metal catalyzed amination of aryl halides and triflates using imines)				
IT	Catalysts				
	Catalysts (imination catalysts; transition metal catalyzed amination of aryl halides and triflates using imines)				
IT	Imination				
	(transition metal catalyzed amination of aryl halides and triflates using imines)				
IT	Transition metals, uses				
	RL: CAT (Catalyst use); USES (Uses)				

- (transition metal catalyzed amination of aryl halides and triflates using imines)
- IT Imines
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(transition metal catalyzed amination of aryl halides and triflates using imines)
- IT Carbonates, miscellaneous
Metal alkoxides
RL: MSC (Miscellaneous)
(transition metal catalyzed amination of aryl halides and triflates using imines)
- IT 3375-31-3, Palladium diacetate 7440-05-3, Palladium, uses 12150-46-8, DPPF 51364-51-3, Tris(dibenzylideneacetone)dipalladium 98327-87-8, BINAP 166330-10-5 255897-36-0
RL: CAT (Catalyst use); USES (Uses)
(transition metal catalyzed amination of aryl halides and triflates using imines)
- IT 32566-86-2P 197144-29-9P 197144-30-2P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(transition metal catalyzed amination of aryl halides and triflates using imines)
- IT 17273-16-4P, N-Diphenylmethylen-4-chloroaniline 35393-20-5P, N-Diphenylmethylen-4-nitroaniline 42834-19-5P, N-Diphenylmethylen-4-methoxyaniline 53847-32-8P, N-Diphenylmethylen-2-chloroaniline 73939-13-6P, N-Diphenylmethylen-2-methoxyaniline 197144-28-8P, N-Diphenylmethylen-4-tert-butylaniline 255835-90-6P, N-Diphenylmethylen-3,5-dimethoxyaniline 255897-33-7P 255897-34-8P, N-Diphenylmethylen-3-(1,3-dioxolan-2-yl)aniline 255897-35-9P, N-Diphenylmethylen-3-fluoroaniline
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(transition metal catalyzed amination of aryl halides and triflates using imines)
- IT 534-17-8, Cesium carbonate 865-48-5
RL: MSC (Miscellaneous)
(transition metal catalyzed amination of aryl halides and triflates using imines)
- IT 100-00-5, 1-Chloro-4-nitrobenzene 104-92-7, 4-Bromoanisole 106-39-8, 4-Bromochlorobenzene 553-94-6, 2,5-Dimethylbromobenzene 578-57-4, 2-Bromoanisole 589-87-7, 4-Bromiodobenzene 619-42-1 623-00-7 626-60-8, 3-Chloropyridine 694-80-4, 2-Bromochlorobenzene 696-62-8, 4-Methoxyiodobenzene 1013-88-3 1073-06-9, 3-Bromofluorobenzene 2398-37-0, 3-Bromoanisole 3972-65-4, 1-Bromo-4-tert-butylbenzene 7051-16-3, 3,5-Dimethoxychlorobenzene 17763-71-2 17789-14-9, 2-(3-Bromophenyl)-1,3-dioxolane 60876-70-2, 4-tert-Butoxybromobenzene 66107-32-2 99747-74-7 107658-28-6 109613-00-5 197144-27-7 255901-58-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(transition metal catalyzed amination of aryl halides and triflates using imines)
- IT 90-04-0P, 2-Methoxyaniline 95-78-3P, 2,5-Dimethylaniline 99-92-3P, 4-Acetylaniline 104-94-9P, 4-Methoxyaniline 106-40-1P, 4-Bromoaniline 134-32-7P, 1-Aminonaphthalene 462-08-8P, 3-Aminopyridine 619-45-4P, 4-Methoxycarbonylaniline 769-92-6P, 4-tert-Butylaniline 873-74-5P, 4-Cyanoaniline 4518-10-9P, 3-Methoxycarbonylaniline 6398-87-4P 197144-31-3P 255901-57-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(transition metal catalyzed amination of aryl halides and triflates using imines)
- RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

- (1) Daicel Chem Ind Ltd; JP 09239275 A 1997 HCAPLUS
 (2) Institut Francais Du Petrole; FR 2474491 A 1981 HCAPLUS
 (3) Syntex Corporation; GB 1047925 A 1966

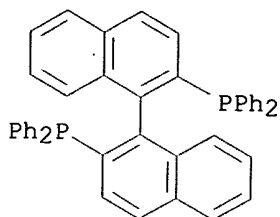
IT 98327-87-8, BINAP

RL: CAT (Catalyst use); USES (Uses)

(transition metal catalyzed amination of aryl halides and triflates using imines)

RN 98327-87-8 HCAPLUS

CN Phosphine, [1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA INDEX NAME)]



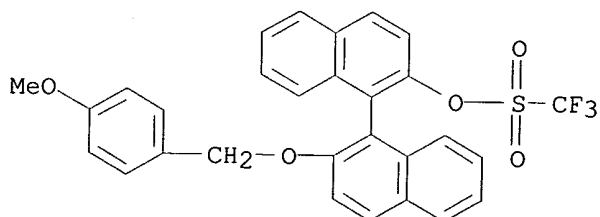
IT 255901-58-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(transition metal catalyzed amination of aryl halides and triflates using imines)

RN 255901-58-7 HCAPLUS

CN Methanesulfonic acid, trifluoro-, 2'--[(4-methoxyphenyl)methoxy][1,1'-binaphthalen]-2-yl ester (9CI) (CA INDEX NAME)



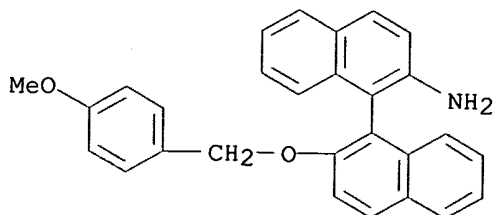
IT 255901-57-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(transition metal catalyzed amination of aryl halides and triflates using imines)

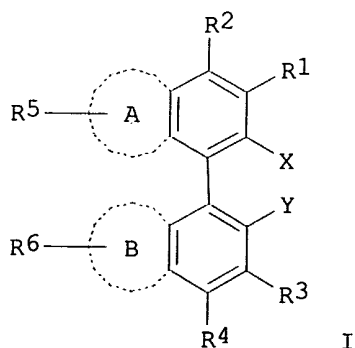
RN 255901-57-6 HCAPLUS

CN [1,1'-Binaphthalen]-2-amine, 2'--[(4-methoxyphenyl)methoxy]- (9CI) (CA INDEX NAME)



DN 132:108101
 TI Biaryl phosphine and amine ligands for improved transition metal-catalyzed processes
 IN Buchwald, Stephen; Old, David W.; Wolfe, John P.; Palucki, Michael; Kamikawa, Ken; Chieffi, Andrew; Sadighi, Joseph P.; Singer, Robert A.; Ahman, Jens
 PA Massachusetts Institute of Technology, USA
 SO PCT Int. Appl., 397 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM C07F009-02
 CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 25
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000002887	A2	20000120	WO 1999-US15450	19990709 <--
	WO 2000002887	A3	20000629		
	W: CA, JP				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 6395916	B1	20020528	US 1998-113478	19980710 <--
	US 6307087	B1	20011023	US 1999-231315	19990113 <--
	CA 2336691	AA	20000120	CA 1999-2336691	19990709 <--
	EP 1097158	A2	20010509	EP 1999-933785	19990709 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2002520328	T2	20020709	JP 2000-559117	19990709 <--
PRAI	US 1998-113478	A	19980710	<--	
	US 1998-196855	A	19981120	<--	
	US 1999-231315	A	19990113		
	US 1999-239024	A	19990127		
	WO 1999-US15450	W	19990709	<--	
OS	MARPAT 132:108101				
GI					



AB The present invention relates to the prepn. of novel biaryl phosphine and amine ligands (I) [wherein A and B = independently fused monocyclic or polycyclic cycloalkyl, cycloalkenyl, aryl, or heterocyclic rings of 4-8 atoms; X = NR₂, PR₂, AsR₂, OR, or SR; Y = NR₂, PR₂, AsR₂, OR, SR, SiR₃, alkyl, or H; R-R₆ = independently H, halogen, (hetero)alkyl, alkenyl, alkynyl, hydroxy, alkoxy, silyloxy, amino, nitro, sulfhydryl, amide, carbonyl, ketone, anhydride, silyl, thioalkyl, ketone, ester, nitrile,

(hetero)aryl, etc.] for transition metals and their use in metal-catalyzed carbon-heteroatom and carbon-carbon bond-forming reactions. Unexpected improvements over the prior art were demonstrated in transition metal-catalyzed aryl amination reactions, Suzuki couplings giving both biaryl and alkylaryl products, arylations and vinylations at the position .alpha. to carbonyl groups, and carbon-oxygen bond formation. The ligands and methods of the invention enable transformations utilizing aryl chlorides and bromides at room temp. at synthetically useful rates with extremely small amts. of catalyst relative to the limiting reagent. For example, coupling of p-chlorobenzonitrile and morpholine was catalyzed by 2.5 mol% Pd2(dba)3, 7.5 mol% of 2-(N,N-dimethylamino)-2'-(dicyclohexylphosphino)biphenyl, and NaOBu-t in DME at room temp. to provide 4-(4-morpholinyl)benzonitrile in 96% yield. Thus, the subject processes provide improvements in many features of the transition metal-catalyzed reactions, including the range of suitable substrates, reaction conditions, and efficiency.

ST biaryl phosphine ammine ligand prepn transition metal catalyst; amination aryl chloride bromide palladium catalysts; Suzuki coupling aryl chloride bromide palladium catalysts; ketone arylation vinylation palladium catalysts; etherification palladium catalysts

IT Amines, preparation

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(arom.; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT Ethers, preparation

Ketones, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(arom.; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT Aryl halides

Aryl halides

RL: RCT (Reactant); RACT (Reactant or reagent)

(aryl chlorides; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT Chlorides, reactions

Chlorides, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(aryl; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT Transition metal complexes

Transition metal complexes

RL: CAT (Catalyst use); USES (Uses)

(phosphine; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT Amination

Amination catalysts

Arylation

Arylation catalysts

Cross-coupling reaction catalysts

Etherification

Etherification catalysts

Suzuki coupling reaction

Vinylation

Vinylation catalysts

(prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

- IT Phosphines
 RL: CAT (Catalyst use); USES (Uses)
 (prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Biaryls
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Aryl bromides
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Phosphines
 Phosphines
 RL: CAT (Catalyst use); USES (Uses)
 (transition metal complexes; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 534-17-8, Dicesium carbonate 3375-31-3, Diacetatopalladium 6476-37-5, Dicyclohexylphenylphosphine 14221-01-3, Tetrakis(triphenylphosphine)palladium 31570-04-4 51364-51-3, Tris(dibenzylideneacetone)dipalladium 54000-83-8, 2,6-Dimethoxyphenyl-di-t-butylphosphine 71042-54-1 74286-11-6 **76189-56-5** 91548-08-2 **100165-88-6** 133545-16-1 136779-28-7 **139139-92-7** **145964-33-6** 149341-34-4 155806-35-2 **213774-71-1** 224311-49-3 247940-06-3 255837-14-0, 2,4,6-Trimethoxyphenyl-di-t-butylphosphine 255837-17-3 255837-19-5 255882-15-6 255882-16-7 255882-17-8 255882-18-9
 RL: **CAT (Catalyst use)**; USES (Uses)
 (catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 698-00-0P 4688-76-0P 18937-92-3P 20837-12-1P, 2-Bromo-2'-methoxy-1,1'-biphenyl 59734-92-8P 75295-57-7P 89291-23-6P 89787-12-2P, 2-Isopropylphenylboronic acid 128796-39-4P, 4-(Trifluoromethyl)phenylboronic acid 224311-57-3P 224311-58-4P 224311-59-5P 251320-87-3P, 2-Bromo-2'-methylbiphenyl 251320-89-5P, 2-Bromo-2'-isopropylbiphenyl 255837-15-1P, 2-Bromo-4'-(trifluoromethyl)biphenyl 255837-16-2P 255837-18-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 213697-53-1P
 RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (prepn. catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 224311-51-7P, 2-(Di-tert-butylphosphino)biphenyl **224311-52-8P** 224311-54-0P 224311-55-1P 251320-85-1P, 2-(Dicyclohexylphosphino)-2'-isopropylbiphenyl 251320-86-2P, 2-(Dicyclohexylphosphino)-2'-methylbiphenyl 255835-81-5P 255835-82-6P 255835-83-7P, 2-(Di-t-butylphosphino)-4'-(trifluoromethyl)biphenyl 255835-84-8P, 2-(Di-t-butylphosphino)-2'-(isopropyl)biphenyl 255835-85-9P 255836-32-9P 255836-65-8P 255836-67-0P 255836-68-1P, 1-[2-(Dicyclohexylphosphino)phenyl]naphthalene 255836-69-2P,

1-[2-(Di-*t*-butylphosphino)phenyl]naphthalene 255882-14-5P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP

(Preparation); USES (Uses)

(prepd. catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT 62-53-3, Benzenamine, reactions 75-97-8 88-05-1 88-69-7 90-04-0
 91-55-4 93-55-0, Propiophenone 95-65-8 95-68-1 95-72-7 96-22-0,
 3-Pentanone 98-54-4 98-80-6 98-86-2, reactions 99-02-5 99-90-1
 99-91-2 100-00-5, 1-Chloro-4-nitrobenzene 100-01-6, reactions
 100-42-5, reactions 100-46-9, Benzenemethanamine, reactions 100-61-8,
 reactions 103-69-5 103-88-8, 4'-Bromoacetanilide 104-92-7 104-94-9
 105-53-3, Diethyl malonate 106-38-7 106-39-8 106-41-2, 4-Bromophenol
 106-43-4 106-49-0, reactions 108-41-8 108-44-1, reactions
 108-91-8, Cyclohexanamine, reactions 108-94-1, Cyclohexanone, reactions
 109-01-3 109-04-6 109-09-1 110-89-4, Piperidine, reactions
 110-91-8, Morpholine, reactions 111-26-2, 1-Hexanamine 111-92-2
 119-61-9, Benzophenone, reactions 120-72-9, Indole, reactions 122-00-9
 122-39-4, Diphenylamine, reactions 123-75-1, Pyrrolidine, reactions
 141-97-9 280-64-8, 9-BBN 392-83-6, 2-Bromobenzotrifluoride 399-52-0
 402-43-7, 4-(Trifluoromethyl)phenyl bromide 460-00-4,
 1-Bromo-4-fluorobenzene 502-42-1, Cycloheptanone 504-02-9,
 1,3-Cyclohexanedione 529-34-0 530-93-8, .beta.-Tetralone 540-88-5,
 tert-Butyl acetate 553-94-6 556-96-7 557-93-7, 2-Bromopropene
 563-80-4 565-69-5 565-80-0 576-22-7 576-26-1 583-53-9,
 1,2-Dibromobenzene 583-55-1, 2-Bromiodobenzene 586-77-6 588-72-7,
 trans-.beta.-Bromostyrene 590-15-8, trans-1-Bromopropene 591-20-8
 592-41-6, 1-Hexene, reactions 615-36-1, 2-Bromoaniline 618-45-1
 618-89-3 619-42-1 623-00-7, 4-Bromobenzonitrile 623-03-0 623-12-1
 624-31-7 626-55-1, 3-Bromopyridine 626-60-8, 3-Chloropyridine
 645-36-3 765-30-0, Cyclopropylamine 766-51-8 766-84-7 778-82-5
 782-17-2 872-31-1, 3-Bromothiophene 873-32-5, 2-Chlorobenzonitrile
 930-29-0, 1-Chlorocyclopentene 931-51-1, Cyclohexylmagnesium chloride
 948-65-2 1003-09-4, 2-Bromothiophene 1013-88-3, Benzophenone imine
 1079-66-9, Chlorodiphenylphosphine 1122-91-4, 4-Bromobenzaldehyde
 1122-95-8 1126-46-1 1450-65-3 1590-08-5 2038-03-1,
 4-Morpholineethanamine 2052-07-5, 2-Bromobiphenyl 2142-68-9,
 2'-Chloroacetophenone 2398-37-0 2635-13-4 2845-89-8 2856-63-5,
 2-Chlorobenzyl cyanide 2905-65-9 3972-65-4, 1-Bromo-4-*t*-butylbenzene
 4079-52-1 4541-32-6 5350-57-2 5619-07-8, DL-Phenylalanine methyl
 ester hydrochloride 5720-06-9 5798-75-4, Ethyl 4-bromobenzoate
 5892-99-9 6781-98-2 7051-16-3 7073-94-1, 2-Bromoisopropylbenzene
 7524-50-7, L-Phenylalanine methyl ester hydrochloride 7598-28-9
 13716-10-4, Chlorodi-*tert*-butylphosphine 13922-41-3, 1-Naphthylboronic
 acid 15499-27-1 16081-16-6 16419-60-6 16523-54-9,
 Chlorodicyclohexylphosphine 17496-14-9, 2-Methylindanone 17763-70-1
 17763-80-3 17789-14-9, 2-(3-Bromophenyl)1,3-dioxolane 17933-03-8
 18982-54-2, 2-Bromobenzyl alcohol 22237-13-4, 4-Ethoxyphenylboronic acid
 22867-74-9 24544-04-5 27505-78-8 27752-24-5 36800-95-0,
 4-Cyanophenyl tosylate 40138-16-7, 2-Formylphenylboronic acid
 41085-43-2, 2-Bromo-3-nitrotoluene 41492-05-1 42371-64-2 53847-33-9
 66107-29-7 66107-32-2 74866-28-7, 2,2'-Dibromo-1,1'-binaphthyl
 100379-00-8 100717-47-3 109613-00-5 112042-84-9 154318-75-9
 157282-19-4 158266-43-4 204841-19-0, 3-Acetylphenylboronic acid
 207611-58-3 255837-20-8 255837-21-9 255837-22-0 255837-23-1
 RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT 78235-91-3P 213697-67-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(starting material; prepn. of biaryl phosphine and amine ligands for

- improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 251320-80-6P, N-(Diphenylmethylene)-2-bromoaniline
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (synthetic product; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 86-26-0P 92-69-3P, 4-Hydroxybiphenyl 92-91-1P, 4-Acetylbiphenyl
 92-93-3P, 4-Nitrobiphenyl 101-70-2P, 4,4'-Dimethoxydiphenylamine
 121-00-6P 613-37-6P, 4-Methoxybiphenyl 620-83-7P 620-93-9P,
 Di-p-tolylamine 644-08-6P, 4-Methylbiphenyl 720-75-2P, Methyl
 4-phenylbenzoate 730-11-0P, 4-Methoxy-4'-nitrodiphenylamine 774-52-7P,
 N-(4-Methylphenyl)piperidine 825-54-7P 825-55-8P, 2-Phenylthiophene
 1208-86-2P 1625-92-9P, 4-t-Butylbiphenyl 2142-66-7P, 2-Acetylbiphenyl
 2920-38-9P, 4-Cyanobiphenyl 2928-43-0P, 2-(Hydroxymethyl)biphenyl
 3077-16-5P, N-(4-Methylphenyl)morpholine 3470-65-3P 3976-34-9P,
 2,6-Dimethylbiphenyl 4036-43-5P 4075-79-0P, N-Acetyl-4-aminobiphenyl
 4316-51-2P, N-(4-Methoxyphenyl)-N,N-diphenylamine 4316-53-4P
 4496-49-5P 4787-76-2P, N-(2-Methoxyphenyl)pyrrolidine 5031-78-7P
 5405-15-2P, N-Benzyl-p-toluidine 5405-19-6P 6574-15-8P,
 N-(4-Nitrophenyl)piperidine 6935-27-9P, N-Benzyl-2-aminopyridine
 7372-85-2P, 2,5-Dimethylbiphenyl 10273-87-7P 10282-31-2P,
 N-(4-Cyanophenyl)morpholine 15359-99-6P 15360-00-6P 16251-99-3P
 16819-50-4P, N-(2,6-Dimethylphenyl)benzylamine 17057-88-4P,
 3,5-Dimethylbiphenyl 17952-07-7P 19853-10-2P, [1,1'-Biphenyl]-2-
 acetonitrile 21218-94-0P 23600-89-7P 23676-05-3P 23699-65-2P,
 N-(3-Acetylphenyl)aniline 23951-29-3P 24255-25-2P,
 N-(2-Pyridyl)morpholine 25539-14-4P 25699-92-7P, N-(4-
 Cyanophenyl)indole 25700-23-6P, N-(3-Pyridyl)indole 27347-14-4P
 31144-33-9P 31603-95-9P, 4-tert-Butyl-1-tert-butyloxybenzene
 34160-16-2P 35393-20-5P, N-(Diphenylmethylene)-4-nitroaniline
 38158-65-5P 38869-05-5P 39253-43-5P 39910-98-0P,
 N-(4-Acetylphenyl)morpholine 50798-94-2P, N-(2-Methoxyphenyl)benzylamine
 50910-08-2P, N-(2-Pyridyl)-N,N-diphenylamine 51580-77-9P 51786-49-3P
 52351-44-7P, N-(4-Methoxyphenyl)-2-phenylindole 54480-44-3P,
 4-Methoxy-4'-(dimethylamino)diphenylamine 54660-04-7P,
 N-(4-Methoxyphenyl)pyrrolidine 55251-46-2P 56052-33-6P 56506-60-6P,
 N-(4-Methylphenyl)hexylamine 56915-80-1P, 1-(3-Acetylphenyl)-4-
 methylpiperazine 60893-66-5P 61394-81-8P 62787-14-8P 62787-15-9P
 62790-83-4P 62790-85-6P 68856-26-8P 70945-85-6P 75201-55-7P
 75934-30-4P 76650-29-8P, 4-Acetyl-3'-methylbiphenyl 76708-72-0P
 76708-78-6P, 2,5,3'-Trimethylbiphenyl 77422-28-7P 81693-80-3P,
 4-Hexylanisole 82749-62-0P 83188-35-6P 84736-47-0P,
 N-(4-t-Butylphenyl)morpholine 84736-54-9P, 2-(4-Methoxyphenyl)-3-
 pentanone 84839-92-9P 84839-93-0P 91949-95-0P, 4-
 Isopropoxybenzonitrile 92495-53-9P, 4-Methyl-2'-methoxybiphenyl
 92670-29-6P, N-(3-Pyridyl)morpholine 93597-01-4P, N-(4-
 Methoxyphenyl)indole 94540-42-8P 94959-58-7P 97053-04-8P
 97413-60-0P 114081-08-2P 114772-53-1P 116267-90-4P,
 N-(3-Thiophenyl)-N,N-diphenylamine 123324-87-8P 124043-95-4P
 129644-26-4P 137445-01-3P 138900-16-0P, N-(4-Fluorophenyl)indole
 138900-19-3P 146803-96-5P 167283-32-1P, N-(4-Methylphenyl)indole
 171092-38-9P, 3-(3-Acetylphenyl)pyridine 172878-95-4P 174307-96-1P
 175696-73-8P, N-(3-Cyanophenyl)pyrrolidine 179487-70-8P 180336-54-3P,
 N-(2,5-Dimethylphenyl)-N-methylaniline 183135-51-5P,
 N-Methyl-N-(3-pyridyl)aniline 183135-52-6P 185259-34-1P,
 N-(4-t-Butylphenyl)piperidine 188026-55-3P, N,N-Dibutyl-4-t-butylaniline
 188026-64-4P, N-Ethyl-N-(3,5-dimethylphenyl)aniline 188026-74-6P
 196604-19-0P 196604-21-4P 196604-24-7P 197172-67-1P 197172-69-3P
 197640-99-6P 202802-70-8P 211292-60-3P 211292-66-9P,
 2,6-Diisopropyl-2',6'-dimethyldiphenylamine 212382-74-6P 213014-13-2P
 213697-51-9P 213697-52-0P, 2,6-Dimethyl-N-hexylaniline 213697-65-5P,

1,1-Bis(4-methylphenyl)-3-methyl-2-butanone 213697-66-6P 215394-88-0P
 223248-27-9P 223655-23-0P 224311-62-0P 224311-63-1P 224311-65-3P
 224311-66-4P 224311-67-5P 224311-68-6P 224311-69-7P 224311-70-0P
 224311-72-2P 224311-73-3P 224311-74-4P 224311-75-5P 224311-76-6P
 226569-78-4P 226917-75-5P, N-(4-Cyanophenyl)hexylamine 247940-07-4P,
 N-Methyl-N-(3,5-dimethoxyphenyl)aniline 247940-08-5P 251320-76-0P
 251320-77-1P, 4-Formyl-4'-ethoxybiphenyl 251320-78-2P 251320-79-3P
 251320-81-7P, 3-Acetyl-3',5'-dimethoxybiphenyl 251320-82-8P
 251320-83-9P 251320-84-0P, 2-Methoxy-2'-acetylbiiphenyl 253768-96-6P,
 N-(3-Cyanophenyl)benzylamine 255835-86-0P 255835-87-1P 255835-88-2P
 255835-89-3P 255835-90-6P 255835-91-7P, N-(2,6-Dimethylphenyl)morpholine 255835-92-8P 255835-93-9P,
 N-(4-t-Butylphenyl)benzylamine 255835-94-0P, N-(3,4-Dimethylphenyl)pyrrolidine 255835-95-1P, 2-Methoxy-4'-cyanodiphenylamine 255835-96-2P 255835-97-3P 255835-98-4P 255835-99-5P 255836-00-1P
 255836-01-2P 255836-02-3P 255836-04-5P, N-(2-Methoxyphenyl)-N-(3-methoxyphenyl)-N-(4-methoxyphenyl)amine 255836-06-7P,
 N-(4-Dimethylaminophenyl)-N-(4-methoxyphenyl)-N-(3-methylphenyl)amine 255836-08-9P, N-(2,4-Dimethylphenyl)-N-(4-methoxyphenyl)-N-(3-methylphenyl)amine 255836-10-3P 255836-12-5P 255836-14-7P,
 N-(4-Butylphenyl)-N-(4-methoxyphenyl)-N-(4-methylphenyl)amine 255836-15-8P, N-(2,5-Dimethylphenyl)-N-(3,5-dimethylphenyl)-N-(4-methylphenyl)amine 255836-17-0P 255836-19-2P, N-(4-tert-Butylphenyl)indole 255836-21-6P 255836-23-8P, N-Cyclopropyl-4-tert-butylaniline 255836-25-0P, N-Cyclopropyl-2,5-dimethylaniline 255836-28-3P 255836-30-7P 255836-36-3P 255836-38-5P 255836-39-6P
 255836-41-0P 255836-43-2P 255836-44-3P 255836-45-4P, 2-Methyl-4-(4-butylphenyl)-3-pentanone 255836-46-5P 255836-48-7P
 255836-50-1P 255836-52-3P 255836-54-5P, 2-(3-Hydroxyphenyl)-3-pentanone 255836-56-7P, 2,4-Dimethyl-2-(4-t-butylphenyl)-3-pentanone 255836-57-8P 255836-59-0P 255836-61-4P 255836-63-6P 255836-70-5P,
 N-(4-t-Butylphenyl)-2-phenylindole 255836-72-7P 255836-74-9P, N-(3,5-Dimethylphenyl)-2,3-dimethylindole 255836-76-1P,
 N-(4-t-Butylphenyl)-2,3,7-trimethylindole 255836-78-3P 255836-80-7P, N-(2-Pyridyl)-7-ethylindole 255836-82-9P, N-(3,5-Dimethylphenyl)-7-ethylindole 255836-84-1P 255836-86-3P 255836-88-5P 255836-90-9P
 255836-92-1P 255836-94-3P 255836-95-4P 255836-96-5P 255836-97-6P
 255836-98-7P 255836-99-8P 255837-00-4P 255837-01-5P 255837-02-6P
 255837-03-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthetic product; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT 255837-04-8P 255837-05-9P 255837-06-0P 255837-07-1P 255837-08-2P
 255837-09-3P 255837-10-6P 255837-11-7P 255837-12-8P 255837-13-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthetic product; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

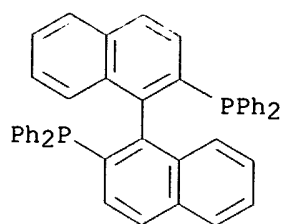
IT 76189-56-5 100165-88-6 139139-92-7
 145964-33-6 213774-71-1

RL: CAT (Catalyst use); USES (Uses)

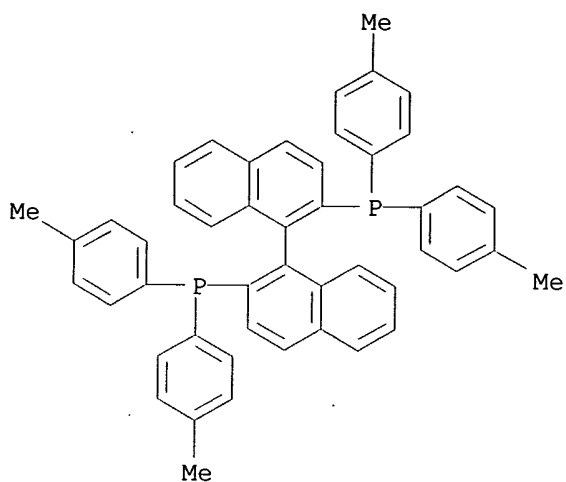
(catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

RN 76189-56-5 HCAPLUS

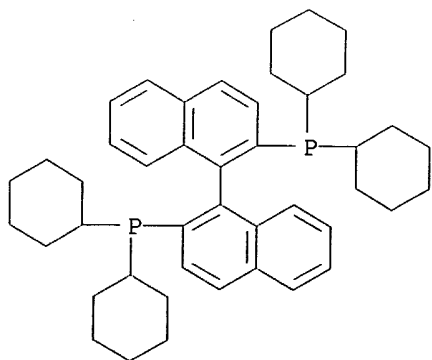
CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA INDEX NAME)



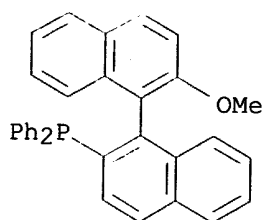
RN 100165-88-6 HCAPLUS
 CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[bis(4-methylphenyl)-
 (9CI) (CA INDEX NAME)



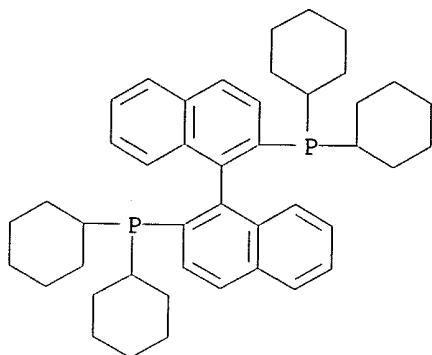
RN 139139-92-7 HCAPLUS
 CN Phosphine, (1R)-[1,1'-binaphthalene]-2,2'-diylbis[dicyclohexyl- (9CI) (CA
 INDEX NAME)



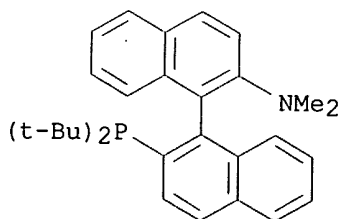
RN 145964-33-6 HCAPLUS
 CN Phosphine, [(1R)-2-methoxy[1,1'-binaphthalen]-2-yl]diphenyl- (9CI) (CA
 INDEX NAME)



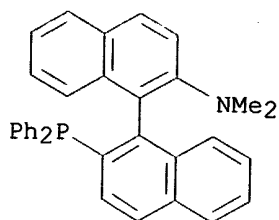
RN 213774-71-1 HCAPLUS
 CN Phosphine, [1,1'-binaphthalene]-2,2'-diylbis[dicyclohexyl- (9CI) (CA INDEX NAME)]



IT 224311-52-8P 255882-14-5P
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (prepd. catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
 RN 224311-52-8 HCAPLUS
 CN [1,1'-Binaphthalen]-2-amine, 2'-[bis(1,1-dimethylethyl)phosphino]-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 255882-14-5 HCAPLUS
 CN [1,1'-Binaphthalen]-2-amine, 2'-(diphenylphosphino)-N,N-dimethyl- (9CI) (CA INDEX NAME)



L34 ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1999:566015 HCAPLUS
 DN 131:199501
 TI Transition metal-catalyzed arylation of hydrazines, hydrazones,
 hydroxylamines, and oximes using activated aromatic compounds.
 IN **Buchwald, Stephen L.**; Wagaw, Seble; Geis, Oliver
 PA Massachusetts Institute of Technology, USA
 SO PCT Int. Appl., 97 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM C07C243-00
 CC 25-5 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 27
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9943643	A2	19990902	WO 1999-US4217	19990226 <--
	WO 9943643	A3	19991021		
	W: CA, JP				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 6235936	B1	20010522	US 1998-30936	19980226 <--
	CA 2322194	AA	19990902	CA 1999-2322194	19990226 <--
	EP 1058678	A2	20001213	EP 1999-908515	19990226 <--
	EP 1058678	B1	20021211		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2002504535	T2	20020212	JP 2000-533402	19990226 <--
	AT 229499	E	20021215	AT 1999-908515	19990226 <--
	US 2001031894	A1	20011018	US 2001-765072	20010118 <--
	US 6465693	B2	20021015		
PRAI	US 1998-30936	A	19980226	<--	
	US 1998-55557	A	19980406	<--	
	WO 1999-US4217	W	19990226		
OS	CASREACT 131:199501				
AB	Hydrazines, hydrazones, hydroxylamines, and oximes were arylated using activated arom. compds. and transition metal catalysts. Thus, PhNHNH2, 4-BrC6H4Me, Pd(OAc)2, BINAP, NaOCMe3, and (Me2CH)2NH were heated together at 80.degree. for 1 h; (CF3CO)2O and Et3N were added to the residue in CH2Cl2 to give 70% N-phenyl-N-4-tolyl-N'-trifluoroacetic hydrazide.				
ST	arylation hydrazine hydrazone hydroxylamine oxime transition metal catalyst; vinylation hydrazine hydrazone hydroxylamine oxime transition metal catalyst				
IT	Arylation catalysts Vinylation catalysts (transition metal compds., phosphines, bases; transition metal-catalyzed arylation of hydrazines, hydrazones, hydroxylamines, and oximes using activated arom. compds.)				
IT	Arylation Vinylation				

- (transition metal-catalyzed arylation of hydrazines, hydrazones, hydroxylamines, and oximes using activated arom. compds.)
- IT Transition metal compounds
 RL: CAT (Catalyst use); USES (Uses)
 (transition metal-catalyzed arylation of hydrazines, hydrazones, hydroxylamines, and oximes using activated arom. compds.)
- IT Hydrazones
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (transition metal-catalyzed arylation of hydrazines, hydrazones, hydroxylamines, and oximes using activated arom. compds.)
- IT Oximes
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (transition metal-catalyzed arylation of hydrazines, hydrazones, hydroxylamines, and oximes using activated arom. compds.)
- IT 3375-31-3, Palladium diacetate 7439-88-5D, Iridium, compds., uses 7439-89-6D, Iron, compds., uses 7440-02-0D, Nickel, compds., uses 7440-05-3D, Palladium, compds., uses 7440-06-4D, Platinum, compds., uses 7440-16-6D, Rhodium, compds., uses 7440-18-8D, Ruthenium, compds., uses 7440-48-4D, Cobalt, compds., uses 7440-50-8D, Copper, compds., uses 76189-56-5 161265-03-8 166330-10-5
 RL: CAT (Catalyst use); USES (Uses)
 (transition metal-catalyzed arylation of hydrazines, hydrazones, hydroxylamines, and oximes using activated arom. compds.)
- IT 40113-76-6P 40594-87-4P 210536-89-3P 210536-91-7P 240482-58-0P 240482-64-8P 240482-68-2P 240482-69-3P
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (transition metal-catalyzed arylation of hydrazines, hydrazones, hydroxylamines, and oximes using activated arom. compds.)
- IT 606-88-2P 30769-69-8P 58263-75-5P 226065-35-6P 240482-52-4P 240482-53-5P 240482-54-6P 240482-55-7P 240482-56-8P 240482-57-9P 240482-67-1P 240482-70-6P 240482-71-7P
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (transition metal-catalyzed arylation of hydrazines, hydrazones, hydroxylamines, and oximes using activated arom. compds.)
- IT 57-14-7, N,N-Dimethylhydrazine 78-93-3, 2-Butanone, reactions 90-11-9, 1-Bromonaphthalene 90-90-4, 4-Bromobenzophenone 92-66-0, 4-Bromobiphenyl 96-22-0, 3-Pentanone 100-39-0, Benzyl bromide 100-46-9, Benzylamine, reactions 100-63-0, Phenylhydrazine 104-92-7, 4-Bromoanisole 106-38-7, 4-Bromotoluene 106-39-8, 4-Chlorobromobenzene 106-49-0, p-Toluidine, reactions 108-86-1, Bromobenzene, reactions 108-94-1, Cyclohexanone, reactions 111-71-7, Heptanal 122-66-7, 1,2-Diphenylhydrazine 123-76-2, Levulinic acid 302-01-2D, Hydrazine, compds., reactions 402-43-7, 4-Bromobenzotrifluoride 407-25-0, Trifluoroacetic anhydride 530-47-2, 1,1-Diphenylhydrazine hydrochloride 556-96-7, 5-Bromo-m-xylene 578-57-4, 2-Bromoanisole 591-78-6, 2-Hexanone 626-55-1, 3-Bromopyridine 694-80-4, 2-Chlorobromobenzene 823-85-8, 4-Fluorophenylhydrazine hydrochloride 870-46-2, tert-Butyl carbazate 2859-78-1, 4-Bromoveratrole 5350-57-2, Benzophenone hydrazone 6156-08-7, Cyclohexanone hydrazone 6952-59-6, 3-Bromobenzonitrile 7699-31-2, 1,2-Diethylhydrazine dihydrochloride 7803-49-8D, Hydroxylamine, compds., reactions 98327-87-8, Binap 240482-76-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (transition metal-catalyzed arylation of hydrazines, hydrazones, hydroxylamines, and oximes using activated arom. compds.)
- IT 36684-65-8P 55542-85-3P 102173-26-2P 107455-62-9P 110178-49-9P 124043-95-4P 240482-60-4P 240482-63-7P 240482-65-9P 240482-72-8P 240482-73-9P 240482-74-0P 240482-75-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (transition metal-catalyzed arylation of hydrazines, hydrazones, hydroxylamines, and oximes using activated arom. compds.)

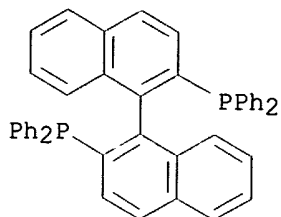
IT 76189-56-5

RL: CAT (Catalyst use); USES (Uses)

(transition metal-catalyzed arylation of hydrazines, hydrazones, hydroxylamines, and oximes using activated arom. compds.)

RN 76189-56-5 HCAPLUS

CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA INDEX NAME)



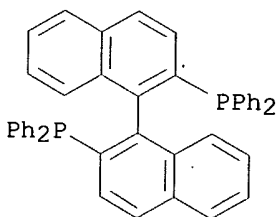
IT 98327-87-8, Binap

RL: RCT (Reactant); RACT (Reactant or reagent)

(transition metal-catalyzed arylation of hydrazines, hydrazones, hydroxylamines, and oximes using activated arom. compds.)

RN 98327-87-8 HCAPLUS

CN Phosphine, [1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA INDEX NAME)



L34 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1998:577201 HCAPLUS

DN 129:275663

TI A Highly Active Catalyst for Palladium-Catalyzed Cross-Coupling Reactions: Room-Temperature Suzuki Couplings and Amination of Unactivated Aryl Chlorides

AU Old, David W.; Wolfe, John P.; Buchwald, Stephen L.

CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

SO Journal of the American Chemical Society (1998), 120(37), 9722-9723

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

CC 25-1 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

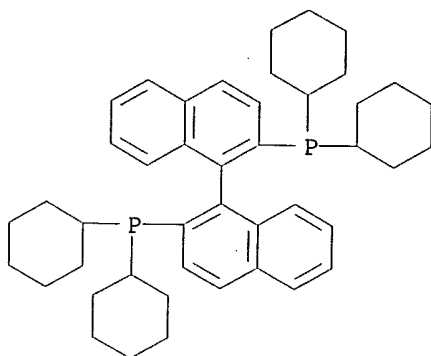
OS CASREACT 129:275663

AB Pd2(dba)3 and ligand 2-(dicyclohexylphosphino)-2'-(dimethylamino)biphenyl catalyzed the amination of aryl chloride or bromides at room temp. Also, Pd2(dba)3 or Pd(OAc)2 and ligand 2-(dicyclohexylphosphino)-2'-(dimethylamino)biphenyl catalyzed the Suzuki coupling of aryl chloride or bromides with boron reagents at room temp.

ST palladium catalyst cross coupling reaction; amination aryl chloride

- bromide palladium catalyst; Suzuki coupling aryl chloride bromide
 IT 3375-31-3, Palladium diacetate 51364-51-3, Pd2(DBA)3 213774-71-1
 RL: CAT (Catalyst use); USES (Uses)
 (palladium-catalyzed Suzuki coupling reactions or amination of aryl chlorides or aryl bromides)
- IT 213697-53-1P
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (palladium-catalyzed Suzuki coupling reactions or amination of aryl chlorides or aryl bromides)
- IT 95-72-7 98-80-6 99-90-1 99-91-2 100-46-9, Benzylamine, reactions 100-61-8, reactions 106-38-7 106-43-4 106-49-0, p-Toluidine, reactions 110-91-8, Morpholine, reactions 111-26-2, Hexylamine 111-92-2, Dibutylamine 553-94-6 556-96-7 563-80-4 565-69-5 576-22-7 583-55-1, 2-Bromiodobenzene 619-42-1 623-03-0 623-12-1 698-00-0 1126-46-1 5720-06-9 16523-54-9, Chlorodicyclohexylphosphine 17933-03-8 42371-64-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (palladium-catalyzed Suzuki coupling reactions or amination of aryl chlorides or aryl bromides)
- IT 89291-23-6P 213697-67-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (palladium-catalyzed Suzuki coupling reactions or amination of aryl chlorides or aryl bromides)
- IT 613-37-6P, 4-Methoxybiphenyl 644-08-6P, 4-Methylbiphenyl 720-75-2P, Methyl 4-biphenylcarboxylate 5405-15-2P 10282-31-2P 17057-88-4P, 3,5-Dimethylbiphenyl 23676-05-3P 27347-14-4P 31144-33-9P 38158-65-5P 39253-43-5P 39910-98-0P 55251-46-2P 76650-29-8P 76708-78-6P 81693-80-3P 82749-62-0P 92495-53-9P 174307-96-1P 180336-54-3P 197172-67-1P 213697-51-9P 213697-52-0P 213697-65-5P 213697-66-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (palladium-catalyzed Suzuki coupling reactions or amination of aryl chlorides or aryl bromides)
- RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
 RE
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 - (2) Beller, M; Angew Chem, Int Ed Engl 1995, V34, P1848 HCAPLUS
 - (3) Bumagin, N; Tetrahedron 1997, V53, P14437 HCAPLUS
 - (4) Campi, E; J Chem Soc, Chem Commun 1994, P2395 HCAPLUS
 - (5) Cornils, B; Org Process Res Dev 1998, V2, P121 HCAPLUS
 - (6) Driver, M; J Am Chem Soc 1996, V118, P7217 HCAPLUS
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 - (14) Mitchell, M; Tetrahedron Lett 1991, V32, P2273 HCAPLUS
 - (15) Miyaaura, N; J Am Chem Soc 1989, V111, P314 HCAPLUS
 - (16) Nishiyama, M; Tetrahedron Lett 1998, V39, P617 HCAPLUS
 - (17) Palucki, M; J Am Chem Soc 1997, V119, P11108 HCAPLUS
 - (18) Reddy, N; Tetrahedron Lett 1997, V38, P4807 HCAPLUS
 - (19) Riermeier, T; Top Catal 1997, V4, P301
 - (20) Saito, S; J Org Chem 1997, V62, P8024 HCAPLUS
 - (21) Shen, W; Tetrahedron Lett 1997, V38, P5575 HCAPLUS
 - (22) Suzuki, A; Metal-Catalyzed Cross-Coupling Reactions, Chapter 2 1998
 - (23) Uenishi, J; J Am Chem Soc 1987, V109, P4756 HCAPLUS
 - (24) Wolfe, J; Acc Chem Res, in press 1996
 - (25) Wolfe, J; J Am Chem Soc 1996, V118, P7215 HCAPLUS
 - (26) Wolfe, J; J Am Chem Soc 1997, V119, P6054 HCAPLUS

- (27) Wolfe, J; J Org Chem 1997, V62, P6066 HCAPLUS
 (28) Wright, S; J Org Chem 1994, V59, P6095 HCAPLUS
 (29) Yamamoto, T; Tetrahedron Lett 1998, V39, P2367 HCAPLUS
 (30) Zhang, X; J Chem Soc, Perkin Trans 1 1994, P2309 HCAPLUS
 IT 213774-71-1
 RL: CAT (Catalyst use); USES (Uses)
 (palladium-catalyzed Suzuki coupling reactions or amination of aryl
 chlorides or aryl bromides)
 RN 213774-71-1 HCAPLUS
 CN Phosphine, [1,1'-binaphthalene]-2,2'-diylbis[dicyclohexyl- (9CI) (CA
 INDEX NAME)



- L34 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1998:431153 HCAPLUS
 DN 129:136056
 TI A Palladium-Catalyzed Strategy for the Preparation of Indoles: A Novel
 Entry into the Fischer Indole Synthesis
 AU Wagaw, Seble; Yang, Bryant H.; Buchwald, Stephen L.
 CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge,
 MA, 02139, USA
 SO Journal of the American Chemical Society (1998), 120(26),
 6621-6622
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
 AB A Fischer indole synthesis was accomplished by Pd-catalyzed cross coupling
 of benzophenone hydrazone with aryl bromides to furnish N-arylhydrazones,
 followed by hydrolysis in presence of a ketone. Purifn. of the
 intermediate hydrazone was not necessary. The catalyst system included
 Pd(OAc)2 and either (S)- or (.+.-)-BINAP.
 ST Fischer indole synthesis palladium catalyst; cross coupling benzophenone
 hydrazone aryl bromide
 IT Fischer indole synthesis
 (palladium-catalyzed Fischer indole synthesis)
 IT Cross-coupling reaction
 Cross-coupling reaction catalysts
 (palladium-catalyzed cross coupling of benzophenone hydrazone with aryl
 bromides)
 IT Aryl bromides
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (palladium-catalyzed cross coupling of benzophenone hydrazone with aryl
 bromides)
 IT Hydrazones
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(prepn. of N-arylhydrazones by palladium-catalyzed cross coupling of benzophenone hydrazone with aryl bromides)

IT 3375-31-3, Palladium diacetate 76189-56-5, (S)-BINAP 98327-87-8, BINAP

RL: CAT (Catalyst use); USES (Uses)

(palladium-catalyzed Fischer indole synthesis)

IT 90-11-9, 1-Bromonaphthalene 92-66-0, 4-Bromobiphenyl 96-22-0, Diethyl ketone 98-86-2, Acetophenone, reactions 106-38-7, p-Bromotoluene 106-39-8, p-Bromochlorobenzene 108-94-1, Cyclohexanone, reactions 111-13-7, 2-Octanone 123-76-2 402-43-7, 4-Bromo(trifluoromethyl)benzene 556-96-7, 5-Bromo-m-xylene 563-80-4, Isopropyl methyl ketone 591-78-6, 2-Hexanone 2398-37-0, 3-Bromoanisole 2859-78-1, 4-Bromoveratrole 5350-57-2, Benzophenone hydrazone 6156-08-7, Cyclohexanone hydrazone 72530-28-0, 2-Octanone hydrazone

RL: RCT (Reactant); RACT (Reactant or reagent)

(palladium-catalyzed Fischer indole synthesis)

IT 40113-76-6P 40594-87-4P 40594-88-5P 210536-89-3P 210536-90-6P 210536-91-7P 210536-92-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(palladium-catalyzed Fischer indole synthesis)

IT 33555-17-8P 34601-58-6P 36684-65-8P 55542-85-3P 110178-49-9P 119266-78-3P 210536-93-9P 210536-94-0P 210536-95-1P 210536-96-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(palladium-catalyzed Fischer indole synthesis)

IT 865-48-5, tert-Butanol sodium salt

RL: NUU (Other use, unclassified); USES (Uses)

(prepn. of)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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- (2) Driver, M; J Am Chem Soc 1996, V118, P7217 HCAPLUS
- (3) Gore, P; Nature 1949, V164, P835 HCAPLUS
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- (5) Hughes, D; Org Prep Proced Int 1993, V25, P607 HCAPLUS
- (6) Mann, G; J Am Chem Soc 1998, V120, P827 HCAPLUS
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- (10) Sundberg, R; Indoles 1996
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- (13) Wolfe, J; Acc Chem Res Submitted for publication
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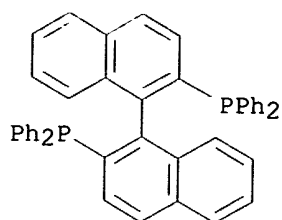
IT 76189-56-5, (S)-BINAP 98327-87-8, BINAP

RL: CAT (Catalyst use); USES (Uses)

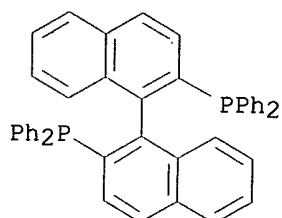
(palladium-catalyzed Fischer indole synthesis)

RN 76189-56-5 HCAPLUS

CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA INDEX NAME)]

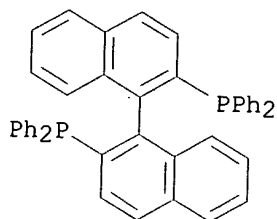


RN 98327-87-8 HCAPLUS
 CN Phosphine, [1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA INDEX NAME)

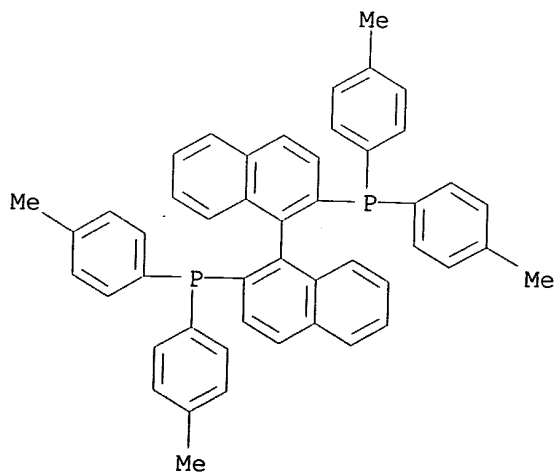


L34 ANSWER 7 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1997:720450 HCAPLUS
 DN 127:331243
 TI Palladium-Catalyzed .alpha.-Arylation of Ketones
 AU **Palucki, Michael; Buchwald, Stephen L.**
 CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
 SO Journal of the American Chemical Society (1997), 119(45), 11108-11109
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 29
 OS CASREACT 127:331243
 AB The combination of Pd2(dba)3 and Tol-BINAP or BINAP in the presence of NaOBu-t catalyzes the reaction of aryl bromides with ketones to give .alpha.-aryl ketones in moderate to high yields. The regioselectivity of arylation of ketones contg. .alpha.,.alpha.'-hydrogens is high: Me > methylene .mchgt. methine. The degree of regioselectivity was found to be independent of the acidity of the .alpha.-hydrogen.
 ST palladium catalyzed arylation ketone
 IT Regiochemistry
 (of palladium-catalyzed arylation of ketones by aryl bromides)
 IT Arylation
 Arylation catalysts
 (palladium-catalyzed .alpha.-arylation of ketones by aryl bromides)
 IT Aryl bromides
 Ketones, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (palladium-catalyzed .alpha.-arylation of ketones by aryl bromides)
 IT 51364-51-3, Tris(dibenzylideneacetone)dipalladium 98327-87-8, BINAP 99646-28-3 100165-88-6
 RL: CAT (Catalyst use); USES (Uses)
 (palladium-catalyzed .alpha.-arylation of ketones by aryl bromides)

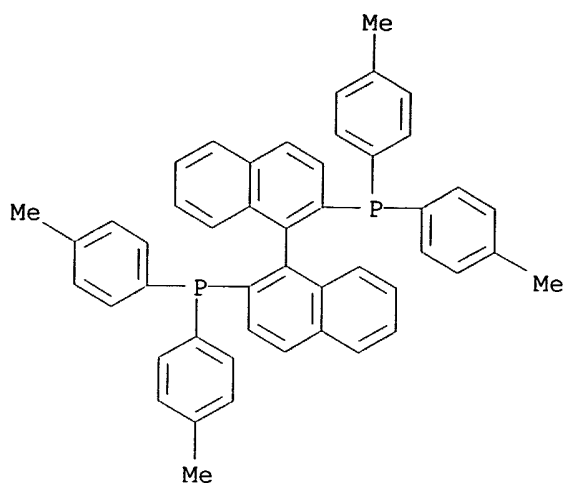
- IT 75-97-8, tert-Butyl methyl ketone 92-66-0 93-55-0, Propiophenone
 99-91-2 100-06-1 106-39-8 108-94-1, Cyclohexanone, reactions
 553-94-6 556-96-7 563-80-4, Isopropyl methyl ketone 565-69-5, Ethyl
 Isopropyl ketone 590-50-1 591-78-6, Butyl methyl ketone 623-00-7,
 p-Bromobenzonitrile 781-35-1 1271-55-2, Acetylferrocene 2398-37-0
 3162-29-6 3972-65-4 5892-99-9 17789-14-9 53847-33-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (palladium-catalyzed .alpha.-arylation of ketones by aryl bromides)
 IT 119046-91-2P 197640-96-3P 197640-97-4P 197640-98-5P 197640-99-6P
 197641-00-2P 197641-01-3P 197641-02-4P 197641-04-6P 197641-05-7P
 197641-06-8P 197641-07-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (palladium-catalyzed .alpha.-arylation of ketones by aryl bromides)
 IT 98327-87-8, BINAP 99646-28-3 100165-88-6
 RL: CAT (Catalyst use); USES (Uses)
 (palladium-catalyzed .alpha.-arylation of ketones by aryl bromides)
 RN 98327-87-8 HCAPLUS
 CN Phosphine, [1,1'-binaphthalene]-2,2'-diylbis[diphenyl]- (9CI) (CA INDEX NAME)



- RN 99646-28-3 HCAPLUS
 CN Phosphine, (1R)-[1,1'-binaphthalene]-2,2'-diylbis[bis(4-methylphenyl)]- (9CI) (CA INDEX NAME)



- RN 100165-88-6 HCAPLUS
 CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[bis(4-methylphenyl)]- (9CI) (CA INDEX NAME)



- L34 ANSWER 8 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1997:595405 HCAPLUS
 DN 127:292927
 TI Improved functional group compatibility in the palladium-catalyzed amination of aryl bromides
 AU **Wolfe, John P.; Buchwald, Stephen L.**
 CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
 SO Tetrahedron Letters (1997), 38(36), 6359-6362
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier
 DT Journal
 LA English
 CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 OS CASREACT 127:292927
 AB Aryl bromides are coupled with amines in the presence of a Pd catalyst and a stoichiometric amt. of Cs carbonate. Using these conditions base-sensitive functional groups, which were incompatible with the authors' previously reported catalytic amination reaction conditions, are well tolerated.
 ST palladium catalyst amination aryl bromide; amine prep
 IT Amination
 Amination catalysts
 (improved functional group compatibility in palladium-catalyzed amination of aryl bromides)
 IT Aryl bromides
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (improved functional group compatibility in palladium-catalyzed amination of aryl bromides)
 IT Amines, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (improved functional group compatibility in palladium-catalyzed amination of aryl bromides)
 IT 3375-31-3, Palladium diacetate 51364-51-3, Tris(dibenzylideneacetone)dipalladium 98327-87-8, BINAP 197241-39-7
 RL: CAT (Catalyst use); USES (Uses)
 (improved functional group compatibility in palladium-catalyzed amination of aryl bromides)
 IT 99-90-1 100-46-9, Benzylamine, reactions 100-61-8, reactions 103-67-3, N-Methylbenzylamine 104-92-7, 4-Bromoanisole 104-94-9, 4-Methoxyaniline 106-49-0, 4-Methylaniline, reactions 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-26-2,

1-Aminohexane 111-92-2 123-75-1, Pyrrolidine, reactions 553-94-6,
 2-Bromo-1,4-dimethylbenzene 586-78-7, 4-Bromonitrobenzene 610-94-6,
 Methyl 2-bromobenzoate 618-89-3, Methyl 3-bromobenzoate 619-42-1,
 Methyl 4-bromobenzoate 623-00-7, 4-Bromocyanobenzene 1122-91-4,
 4-Bromobenzaldehyde 2038-03-1, 4-(2-Aminoethyl)morpholine 3972-65-4,
 4-tert-Butyl-1-bromobenzene 5798-75-4, Ethyl 4-bromobenzoate
 40371-64-0 154607-01-9, 4-Bromo-2-chlorobenzonitrile

RL: RCT (Reactant); RACT (Reactant or reagent)

(improved functional group compatibility in palladium-catalyzed
 amination of aryl bromides)

IT 1204-85-9P 1215-41-4P 6574-15-8P 21971-24-4P 23600-89-7P
 27347-14-4P 65213-46-9P 97053-04-8P 101038-65-7P 158833-49-9P
 185259-34-1P 188026-55-3P 197172-65-9P 197172-67-1P 197172-69-3P
 197173-65-2P 197173-66-3P 197173-67-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

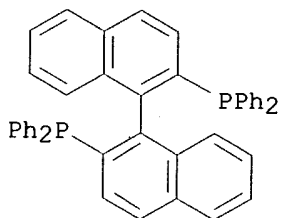
IT 98327-87-8, BINAP

RL: CAT (Catalyst use); USES (Uses)

(improved functional group compatibility in palladium-catalyzed
 amination of aryl bromides)

RN 98327-87-8 HCAPLUS

CN Phosphine, [1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA INDEX
 NAME)



L34 ANSWER 9 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1997:565069 HCAPLUS

DN 127:205161

TI Palladium-Catalyzed Coupling of Optically Active Amines with Aryl Bromides
 AU Wagaw, Seble; Rennels, Roger A.; Buchwald, Stephen L.

CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge,
 MA, 02139, USA

SO Journal of the American Chemical Society (1997), 119(36),
 8451-8458

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

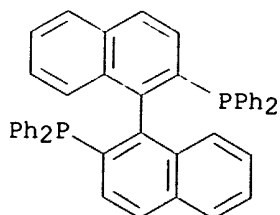
LA English

CC 21-2 (General Organic Chemistry)

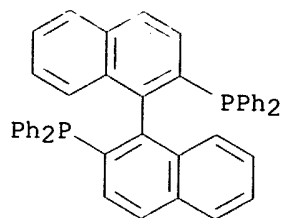
OS CASREACT 127:205161

AB The coupling of enantiomerically enriched amines with aryl bromides
 produces the corresponding N-aryl derivs. The choice of ligand in the
 palladium-catalyzed coupling is crit. to the formation of the anilines
 without loss of enantiomeric purity. While $\text{LnPd} [\text{L} = \text{P}(\text{o-tolyl})_3]$
 successfully catalyzes the intramol. aryl amination of α -substituted
 optically pure amines, intermol. coupling reactions with this catalyst
 system gives racemized products. In contrast, intermol. N-arylations
 employing $\text{LnPd} [\text{L} = (.-.-)\text{-BINAP}]$ gives products in good yields with no
 erosion of enantiopurity. A mechanism for the obsd. racemization is
 proposed. The utility of the intramol. process is demonstrated by the
 synthesis of 3, an intermediate in the formal synthesis of 4, a potent ACE
 inhibitor.

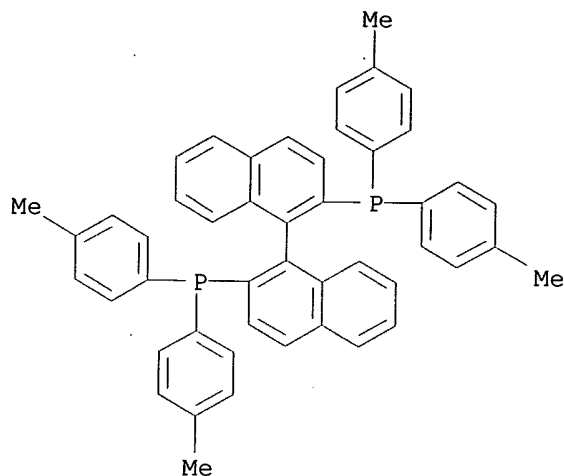
- ST palladium catalyst coupling amine aryl bromide
 IT Coupling reaction catalysts
 Stereochemistry
 (palladium-catalyzed coupling of optically active amines with aryl bromides)
- IT Amines, reactions
 Aryl bromides
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (palladium-catalyzed coupling of optically active amines with aryl bromides)
- IT 603-35-0, Triphenylphosphine, uses 3375-31-3, Palladium diacetate
 3411-48-1, Tris(1-naphthyl)phosphine 4731-65-1, Tris(o-methoxyphenyl)phosphine
 6163-58-2, Tris(o-methylphenyl)phosphine 12150-46-8, DPPF 51364-51-3
 72287-26-4 98327-87-8, BINAP 99326-34-8 136779-28-7
 RL: CAT (Catalyst use); USES (Uses)
 (palladium-catalyzed coupling of optically active amines with aryl bromides)
- IT 82924-03-6P
 RL: PNU (Preparation, unclassified); PREP (Preparation)
 (palladium-catalyzed coupling of optically active amines with aryl bromides)
- IT 90-90-4, 4-Bromobenzophenone 92-66-0, 4-Bromobiphenyl 106-39-8
 109-04-6, 2-Bromopyridine 115-11-7, Isobutylene, reactions 402-43-7
 513-49-5 580-13-2, 2-Bromonaphthalene 583-55-1, o-Iodobromobenzene
 628-20-6, 4-Chlorobutyronitrile 3182-95-4, (S)-Phenylalaninol
 3886-69-9, (R)-.alpha.-Methylbenzylamine 4165-57-5, Bromobenzene-d5
 5913-13-3 5933-40-4 17789-14-9 18698-97-0, 2-Bromophenylacetic acid
 20439-47-8 23356-96-9, (S)-Prolinol 35356-70-8 59347-91-0,
 (S)-2-Phenylpyrrolidine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (palladium-catalyzed coupling of optically active amines with aryl bromides)
- IT 154261-30-0P 194723-99-4P 194724-01-1P 194724-02-2P 194724-09-9P
 194724-26-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (palladium-catalyzed coupling of optically active amines with aryl bromides)
- IT 110592-39-7P 194724-00-0P 194724-03-3P 194724-04-4P 194724-10-2P
 194724-13-5P 194724-16-8P 194724-18-0P 194724-20-4P 194724-22-6P
 194724-24-8P 194724-25-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (palladium-catalyzed coupling of optically active amines with aryl bromides)
- IT 98327-87-8, BINAP
 RL: CAT (Catalyst use); USES (Uses)
 (palladium-catalyzed coupling of optically active amines with aryl bromides)
- RN 98327-87-8 HCAPLUS
 CN Phosphine, [1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA INDEX NAME)]



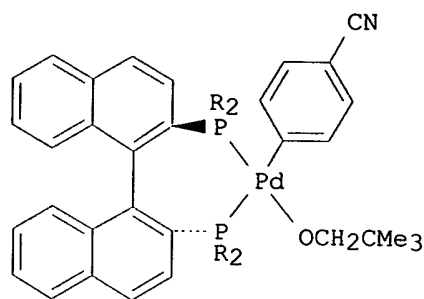
L34 ANSWER 10 OF 19 HCAPLUS COPYRIGHT 2003 ACS
AN 1997:559636 HCAPLUS
DN 127:262475
TI Room temperature catalytic amination of aryl iodides
AU Wolfe, John P.; Buchwald, Stephen L.
CS Department Chemistry, Massachusetts Institute Technology, Cambridge, MA,
02139, USA
SO Journal of Organic Chemistry (1997), 62(17), 6066-6068
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
OS CASREACT 127:262475
AB Mixts. of Pd2(dba)3 and BINAP or Tol-BINAP catalyze the coupling of aryl
iodides with aliph. amines in the presence of stoichiometric amts. of
NaOBu-t and 18-Crown-6 at room temp. in good to excellent yields.
Anilines may be coupled with aryl iodides under similar conditions at 40
degree.C in good yields. For example, the amination of
1-iodo-4-methylbenzene with piperidine gave 1-(4-methylphenyl)piperidine
in 85% yield.
ST amination aryl iodide amine; benzenamine phenyl prepn; phenylmorpholine
phenylpiperidine prepn
IT Iodides, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(arom.; room temp. catalytic amination of aryl iodides)
IT Amination
(room temp. catalytic amination of aryl iodides)
IT 620-84-8P 22148-20-5P 54660-04-7P, N-(4-Methoxyphenyl)pyrrolidine
65489-12-5P 84736-47-0P 87698-82-6P 97053-04-8P 174307-98-3P
196213-26-0P 196213-27-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 51364-51-3, Tris(dibenzylideneacetone)dipalladium 76189-56-5,
(S)-BINAP 99646-28-3
RL: CAT (Catalyst use); USES (Uses)
(room temp. catalytic amination of aryl iodides)
IT 62-53-3, Benzenamine, reactions 95-53-4, 2-Methylaniline, reactions
100-61-8, N-Methylaniline, reactions 104-94-9, 4-Methoxyaniline
110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions
111-26-2, 1-Hexanamine 123-75-1, Pyrrolidine, reactions 583-55-1,
1-Bromo-2-iodobenzene 589-87-7, 1-Bromo-4-iodobenzene 591-18-4,
1-Bromo-3-iodobenzene 624-31-7, 1-Iodo-4-methylbenzene 696-62-8,
1-Iodo-4-methoxybenzene 865-48-5, Sodium tert-butoxide 1122-42-5,
2-Iodo-1,4-dimethylbenzene 35779-04-5 77350-52-8, N,N-Diethyl-4-
iodobenzamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(room temp. catalytic amination of aryl iodides)
IT 31053-03-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(room temp. catalytic amination of aryl iodides)
IT 76189-56-5, (S)-BINAP 99646-28-3
RL: CAT (Catalyst use); USES (Uses)
(room temp. catalytic amination of aryl iodides)
RN 76189-56-5 HCAPLUS
CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA
INDEX NAME)



RN 99646-28-3 HCAPLUS
 CN Phosphine, (1R)-[1,1'-binaphthalene]-2,2'-diylbis[phenyl]-
 (9CI) (CA INDEX NAME)



L34 ANSWER 11 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1997:457099 HCAPLUS
 DN 127:135936
 TI Direct Observation of C-O Reductive Elimination from Palladium Aryl
 Alkoxide Complexes To Form Aryl Ethers
 AU Widenhoefer, Ross A.; Zhong, H. Annita; **Buchwald, Stephen L.**
 CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge,
 MA, 02139, USA
 SO Journal of the American Chemical Society (1997), 119(29),
 6787-6795
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 22
 OS CASREACT 127:135936
 GI



I

- AB Reaction of KOCH₂CMe₃ with [(R)-Tol-BINAP]Pd(p-C₆H₄CN)Br formed [(R)-Tol-BINAP]Pd(p-C₆H₄CN)(OCH₂CMe₃) I (5; R = p-tolyl) in quant. yield (1H NMR spectroscopy). Thermolysis of 5 in THF-d₈ at 47.degree. led to C-O reductive elimination with formation of p-neopentoxymbenzotrile (85 .+- . 2%). A secondary P-C bond-cleavage process gave 4,4'-dimethylbiphenyl (16 .+- . 2%). Kinetic anal. of the decompn. of 5 at 47.degree. in the presence of excess K neopentoxide established the two-term rate law, rate = k[5] + k'[5][KOCH₂CMe₃], where k = 1.50 .+- . 0.07 .times. 10⁻³ s⁻¹ and k' = 6.2 .+- . 0.4 .times. 10⁻³ s⁻¹ M⁻¹, consistent with reductive elimination via competing alkoxide-dependent and alkoxide-independent pathways. Excess KOCH₂CMe₃ exchanged rapidly with the Pd-bound alkoxide ligand of 5 at 47.degree. according to the rate law: rate exchange = k_{ex}[5][KOCH₂CMe₃], where k_{ex} = 1.0 .+- . 0.1 .times. 10² s⁻¹ M⁻¹. Thermolysis of the related Pd p-cyanophenyl alkoxide complexes (P-P)Pd(p-C₆H₄CN)(OR) [P-P = (S)-BINAP, R = CH₂CMe₃; P-P = (R)-Tol-BINAP, R = CHMe₂, CMe₃; P-P = 1,1'-bis(diphenylphosphino)ferrocene (dppf), R = CH₂CMe₃, CMe₃] and (dppf)Pd[o-C₆H₄(CH₂)₂C(Me)₂O] led to aryl ether formation in 46-91% yield.
- ST aryl ether prepn; palladium aryl alkoxide prepn reductive elimination; thermal decompn palladium aryl alkoxide kinetics
- IT Ethers, preparation
- RL: SPN (Synthetic preparation); PREP (Preparation)
(arom.; formation of aryl ethers by reductive elimination from palladium aryl alkoxide complexes)
- IT Bond formation
(carbon-oxygen; in formation of aryl ethers by reductive elimination from palladium aryl alkoxide complexes)
- IT Linear free energy relationship
(for kinetics of thermal decompn. of palladium aryl alkoxide complexes)
- IT Thermal decomposition kinetics
(kinetics of thermal decompn. of palladium aryl alkoxide complexes)
- IT Elimination reaction, coordinative
(reductive; reductive elimination from palladium aryl alkoxide complexes)
- IT 92-52-4P, Biphenyl, preparation 100-47-0P, Benzonitrile, preparation
613-33-2P, 4,4'-Dimethylbiphenyl 630-19-3P, Pivaldehyde 644-08-6P,
4-Methylbiphenyl 79615-68-2P 91949-95-0P 185259-36-3P
- RL: SPN (Synthetic preparation); PREP (Preparation)
(formation of aryl ethers by reductive elimination from palladium aryl alkoxide complexes)
- IT 193001-21-7P 193001-23-9P 193001-25-1P 193001-27-3P 193001-29-5P
193001-31-9P 193001-33-1P 193001-36-4P
- RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and kinetics of thermal decompn. of palladium aryl alkoxide complexes)
- IT 623-00-7, 4-Bromobenzonitrile 865-47-4, Potassium tert-butoxide
1192-96-7, Potassium p-cresolate 3058-39-7, 4-Iodobenzonitrile

6163-58-2, Tri-o-tolylphosphine 6831-82-9, Potassium isopropoxide
 12150-46-8, 1,1'-Bis(diphenylphosphino)ferrocene 51364-51-3
 55553-85-0, Potassium neopentoxide 76189-56-5 99646-28-3
 100165-88-6 183864-59-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of palladium aryl alkoxide complexes)

IT 193001-13-7P 193001-15-9P 193001-17-1P 193001-19-3P 193001-39-7P
 193001-41-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. of palladium aryl alkoxide complexes)

IT 1198-96-5P

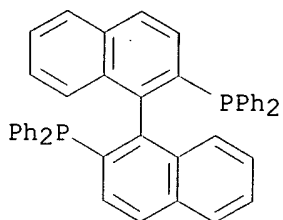
RL: SPN (Synthetic preparation); PREP (Preparation)
 (thermal decompn. of palladium aryl alkoxide complexes)

IT 76189-56-5 99646-28-3 100165-88-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of palladium aryl alkoxide complexes)

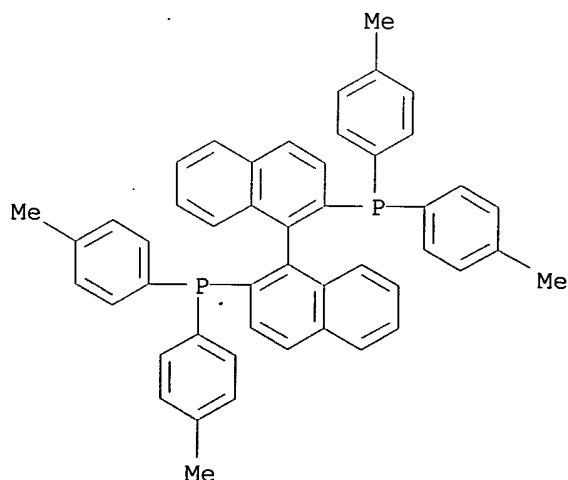
RN 76189-56-5 HCAPLUS

CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA
 INDEX NAME)]



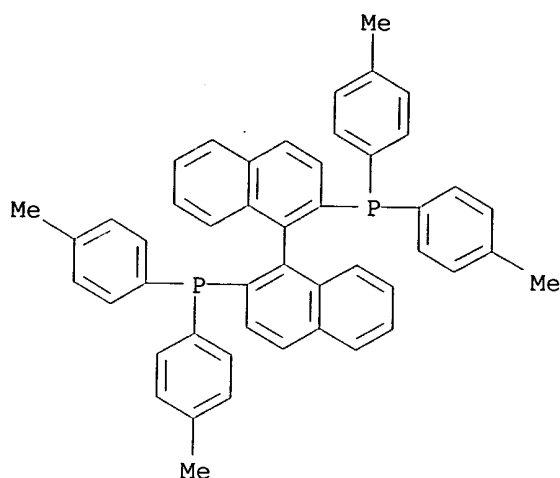
RN 99646-28-3 HCAPLUS

CN Phosphine, (1R)-[1,1'-binaphthalene]-2,2'-diylbis[bis(4-methylphenyl)-
 (9CI) (CA INDEX NAME)]



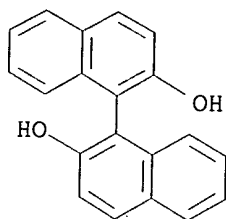
RN 100165-88-6 HCAPLUS

CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[bis(4-methylphenyl)-
 (9CI) (CA INDEX NAME)]



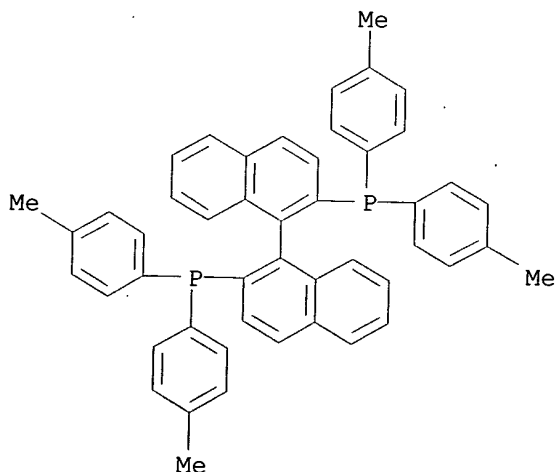
- L34 ANSWER 12 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1997:226494 HCAPLUS
 DN 126:199628
 TI Improved Procedure for the Preparation of Enantiomerically Pure
 Ethylenebis(tetrahydroindenyl)zirconium Derivatives
 AU Chin, Bain; Buchwald, Stephen L.
 CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge,
 MA, MASSACHUSETTS 02139, USA
 SO Journal of Organic Chemistry (1997), 62(7), 2267-2268
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 CC 29-10 (Organometallic and Organometalloidal Compounds)
 OS CASREACT 126:199628
 AB Enantiomerically pure complexes (R,R)-ethylenebis(tetrahydroindenyl)
 Zr(R)-1,1'-binaphth-2,2'-diolate and (S,S)-ethylenebis(tetrahydroindenyl)
 Zr(S)-1,1'-biphen-2,2'-diolate (1d) were prepd. from (rac)-
 ethylenebis(tetrahydroindenyl)zirconium dichloride (1a) and
 (R)-1,1'-binaphth-2,2'-diol. The enantiomer of 1a that did not form a
 binaphthdiolate complex was sepd. as an ethylenebis(tetrahydroindenyl)zirc
 onium bis(4-aminobenzoate) complex and then converted to 1d.
 ST enantiomer ethylenebistetrahydroindenyl zirconium complex prepn; indenyl
 ethylenebistetrahydro zirconium complex enantiomer prepn
 IT Enantiomers
 .(improved procedure for prepn. of enantiomerically pure
 ethylene(tetrahydroindenyl)zirconium derivs.)
 IT Metallocenes
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (zirconocenes; improved procedure for prepn. of enantiomerically pure
 ethylene(tetrahydroindenyl)zirconium derivs.)
 IT 150-13-0, 4-Aminobenzoic acid 1806-29-7, 1,1'-Biphen-2-ol
 18531-94-7, (R)-1,1'-Binaphth-2,2'-diol 100163-29-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (improved procedure for prepn. of enantiomerically pure
 ethylene(tetrahydroindenyl)zirconium derivs.)
 IT 187661-02-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (improved procedure for prepn. of enantiomerically pure
 ethylene(tetrahydroindenyl)zirconium derivs.)
 IT 115857-04-0P 115938-35-7P 123236-85-1P 187757-13-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (improved procedure for prepn. of enantiomerically pure
 ethylene(tetrahydroindenyl)zirconium derivs.)
 IT 18531-94-7, (R)-1,1'-Binaphth-2,2'-diol
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (improved procedure for prepn. of enantiomerically pure
 ethylene(tetrahydroindenyl)zirconium derivs.)
 RN 18531-94-7 HCAPLUS
 CN [1,1'-Binaphthalene]-2,2'-diol, (1R)- (9CI) (CA INDEX NAME)

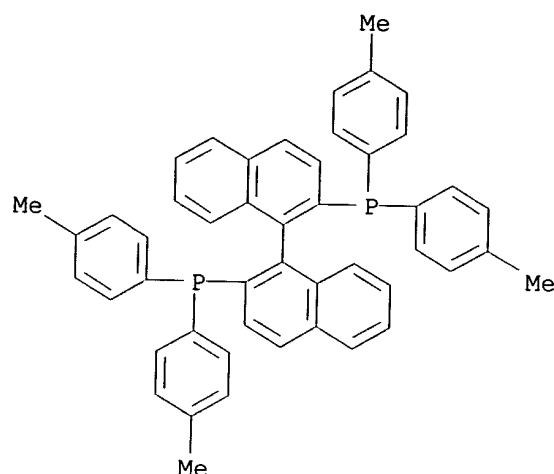


L34 ANSWER 13 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1997:195810 HCAPLUS
 DN 126:250954
 TI Palladium-Catalyzed Intermolecular Carbon-Oxygen Bond Formation: A New
 Synthesis of Aryl Ethers
 AU Palucki, Michael; Wolfe, John P.; Buchwald,
 Stephen L.
 CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge,
 MA, 02139, USA
 SO Journal of the American Chemical Society (1997), 119(14),
 3395-3396
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 OS CASREACT 126:250954
 AB The synthesis of aryl ethers by the intermol. formation of a carbon-oxygen
 bond can be catalyzed by a combination of Pd2(dba)3 or Pd(OAc)2 and
 Tol-BINAP in toluene. This process yields aryl ethers in moderate to good
 yields. While little or no conversion is seen in control reactions run in
 toluene, it was found for some electron-poor aryl bromides that
 nucleophilic arom. substitution could be carried out in DMF in the absence
 of metal catalyst under mild conditions.
 ST palladium catalyst substitution bromoarene alc; aryl ether prepn
 IT Ethers, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (arom.; prepn. of aryl ethers by palladium-catalyzed reaction of aryl
 bromides and alcs.)
 IT Substitution reaction, nucleophilic
 (arom.; uncatalyzed and palladium-catalyzed reaction of aryl bromides
 and alcs.)
 IT Bond formation
 (carbon-oxygen; palladium-catalyzed carbon-oxygen bond formation)
 IT Substitution reaction catalysts
 (nucleophilic, arom.; uncatalyzed and palladium-catalyzed reaction of
 aryl bromides and alcs.)
 IT Alcohols, reactions
 Aryl bromides
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of aryl ethers by palladium-catalyzed reaction of aryl bromides

- and alcs.)
- IT 3375-31-3, Palladium diacetate 51364-51-3, Tris(dibenzylideneacetone)dipalladium 99646-28-3 100165-88-6
 RL: CAT (Catalyst use); USES (Uses)
 (prepn. of aryl ethers by palladium-catalyzed reaction of aryl bromides and alcs.)
- IT 67-56-1, Methanol, reactions 67-63-0, 2-Propanol, reactions 90-11-9, 1-Bromonaphthalene 96-41-3, Cyclopentanol 98-85-1, sec-Phenethyl alcohol 100-51-6, Benzyl alcohol, reactions 108-93-0, Cyclohexanol, reactions 402-43-7 584-02-1, 3-Pentanol 623-00-7, p-Bromobenzonitrile 865-48-5, Sodium tert-butoxide 1564-64-3, 9-Bromoanthracene 2081-44-9 2216-51-5, (-)-Menthol 3972-65-4 154607-01-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of aryl ethers by palladium-catalyzed reaction of aryl bromides and alcs.)
- IT 874-90-8P 21571-62-0P 31603-95-9P 52805-36-4P 91949-95-0P 188527-52-8P 188527-54-0P 188527-60-8P 188527-62-0P 188527-64-2P 188527-66-4P 188527-68-6P 188527-70-0P 188527-72-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of aryl ethers by palladium-catalyzed reaction of aryl bromides and alcs.)
- IT 99646-28-3 100165-88-6
 RL: CAT (Catalyst use); USES (Uses)
 (prepn. of aryl ethers by palladium-catalyzed reaction of aryl bromides and alcs.)
- RN 99646-28-3 HCAPLUS
 CN Phosphine, (1R)-[1,1'-binaphthalene]-2,2'-diylbis[bis(4-methylphenyl)]-(9CI) (CA INDEX NAME)

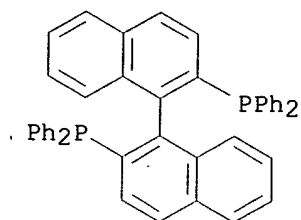


- RN 100165-88-6 HCAPLUS
 CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[bis(4-methylphenyl)]-(9CI) (CA INDEX NAME)

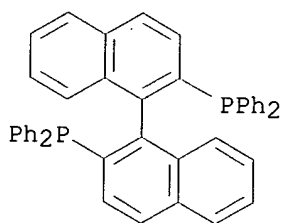


- L34 ANSWER 14 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1997:164910 HCAPLUS
 DN 126:143782
 TI Palladium-Catalyzed Amination of Aryl Triflates
 AU **Wolfe, John P.; Buchwald, Stephen L.**
 CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
 SO Journal of Organic Chemistry (1997), 62(5), 1264-1267
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 CC 21-2 (General Organic Chemistry)
 OS CASREACT 126:143782
 AB The conversion of aryl triflates to the corresponding aniline derivs. was accomplished in moderate to good yield using a catalyst consisting of the combination of palladium acetate (2 mol %) and either BINAP or Tol-BINAP. In contrast to the corresponding palladium-catalyzed amination of aryl bromides and iodides, electronically neutral aryl triflates gave higher yields of arylamines than did electron deficient aryl triflates, presumably due to the increased rate of base-promoted triflate cleavage in electron deficient substrates.
- ST palladium catalyst amination aryl triflate
 IT Amination
 Amination catalysts
 (palladium-catalyzed amination of aryl triflates)
- IT 3375-31-3, Palladium diacetate 51364-51-3, Tris(dibenzylideneacetone)dipalladium 76189-55-4, (R)-BINAP 76189-56-5, (S)-BINAP 99646-28-3 100165-88-6
 RL: CAT (Catalyst use); USES (Uses)
 (palladium-catalyzed amination of aryl triflates)
- IT 62-53-3, Aniline, reactions 103-67-3, N-Methylbenzylamine 109-01-3, 1-Methylpiperazine 109-73-9, Butylamine, reactions 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-26-2, Hexylamine 123-75-1, Pyrrolidine, reactions 177-11-7, 1,4-Dioxo-8-azaspiro[4.5]decane 66107-29-7 66107-32-2 87241-52-9 99747-74-7, 1-Naphthyl triflate 109586-43-8 124643-34-1 154318-75-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (palladium-catalyzed amination of aryl triflates)
- IT 90-30-2P 10282-31-2P 24758-49-4P 54660-04-7P 66797-55-5P 81506-14-1P 114849-77-3P 151696-67-2P 185259-34-1P 186682-66-6P 186682-67-7P 186682-68-8P 186682-69-9P 186682-70-2P 186682-71-3P

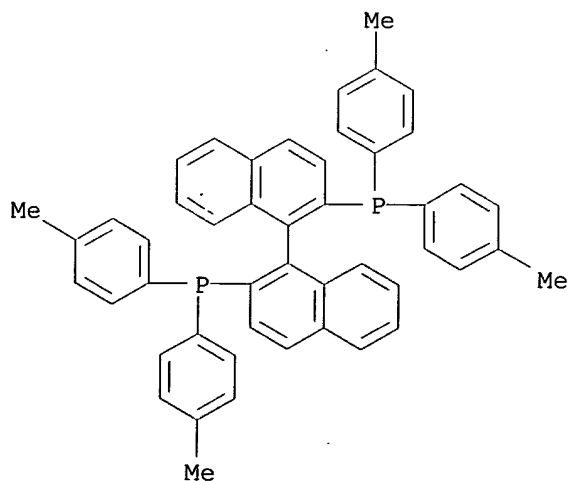
RL: SPN (Synthetic preparation); PREP (Preparation)
 (palladium-catalyzed amination of aryl triflates)
 IT 76189-55-4, (R)-BINAP 76189-56-5, (S)-BINAP
 99646-28-3 100165-88-6
 RL: CAT (Catalyst use); USES (Uses)
 (palladium-catalyzed amination of aryl triflates)
 RN 76189-55-4 HCAPLUS
 CN Phosphine, (1R)-[1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA
 INDEX NAME)



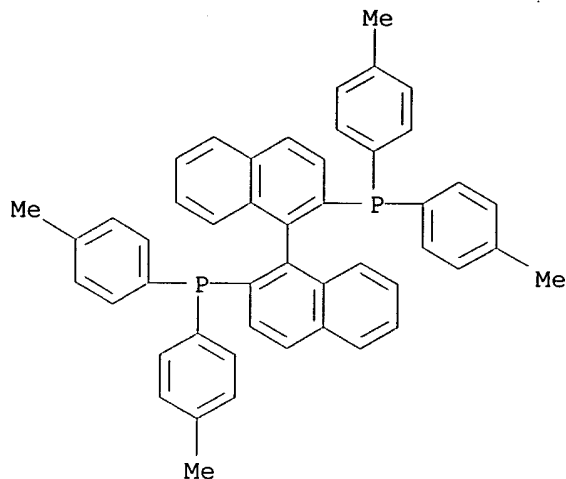
RN 76189-56-5 HCAPLUS
 CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA
 INDEX NAME)



RN 99646-28-3 HCAPLUS
 CN Phosphine, (1R)-[1,1'-binaphthalene]-2,2'-diylbis[bis(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 100165-88-6 HCAPLUS
 CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[bis(4-methylphenyl)- (9CI) (CA INDEX NAME)



- L34 ANSWER 15 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1996:618987 HCAPLUS
 DN 125:328464
 TI The Synthesis of Aminopyridines: A Method Employing Palladium-Catalyzed Carbon-Nitrogen Bond Formation
 AU Wagaw, Seble; **Buchwald, Stephen L.**
 CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
 SO Journal of Organic Chemistry (1996), 61(21), 7240-7241
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
 OS CASREACT 125:328464
 AB Aminopyridines are efficiently synthesized under mild conditions by the cross coupling reaction of 2-, 3-, and 4-bromopyridines with primary and secondary amines utilizing palladium(0) complexes with chelating bis(phosphine) ligands. A variety of aminopyridines were prep'd. including mono-, di-, tri-, and tetra-pyridinylated products.
 ST aminopyridine prepn; pyridine amino prepn; cross coupling bromopyridine amine
 IT Amines, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of aminopyridines by palladium-catalyzed cross coupling of bromopyridines with amines)
 IT Coupling reaction
 Coupling reaction catalysts
 (cross-, prepn. of aminopyridines by palladium-catalyzed cross coupling of bromopyridines with amines)
 IT 3375-31-3, Palladium diacetate 6737-42-4, Dppp 51364-51-3
 98327-87-8, BINAP
 RL: **CAT (Catalyst use)**; USES (Uses)
 (prepn. of aminopyridines by palladium-catalyzed cross coupling of bromopyridines with amines)
 IT 62-53-3, Aniline, reactions 100-61-8, N-Methylaniline, reactions
 103-67-3, N-Methylbenzylamine 108-91-8, Cyclohexylamine, reactions
 109-04-6, 2-Bromopyridine 109-09-1, 2-Chloropyridine 109-76-2,
 1,3-Diaminopropane 110-91-8, Morpholine, reactions 111-26-2,
 Hexylamine 504-29-0, 2-Aminopyridine 626-05-1, 2,6-Dibromopyridine
 626-55-1, 3-Bromopyridine 1121-22-8, trans-1,2-Diaminocyclohexane

5332-24-1, 3-Bromoquinoline 19524-06-2, 4-Bromopyridine hydrochloride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of aminopyridines by palladium-catalyzed cross coupling of
 bromopyridines with amines)

IT 1202-34-2P 2767-91-1P 5051-97-8P 15513-16-3P 20173-75-5P
 24255-25-2P 32405-79-1P 64690-14-8P 92670-29-6P 100051-12-5P
 183135-50-4P 183135-51-5P 183135-52-6P 183135-53-7P 183135-54-8P
 183135-55-9P 183135-56-0P

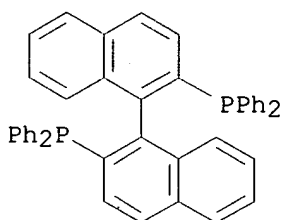
RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of aminopyridines by palladium-catalyzed cross coupling of
 bromopyridines with amines)

IT 98327-87-8, BINAP

RL: CAT (Catalyst use); USES (Uses)
 (prepn. of aminopyridines by palladium-catalyzed cross coupling of
 bromopyridines with amines)

RN 98327-87-8 HCAPLUS

CN Phosphine, [1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA INDEX
 NAME)



L34 ANSWER 16 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1996:616752 HCAPLUS

DN 126:7946

TI Synthesis of Oxygen Heterocycles via a Palladium-Catalyzed C-O
 Bond-Forming Reaction

AU Palucki, Michael; Wolfe, John P.; Buchwald,
 Stephen L.

CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge,
 MA, 02139, USA

SO Journal of the American Chemical Society (1996), 118(42),
 10333-10334

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

CC 27-13 (Heterocyclic Compounds (One Hetero Atom))

OS CASREACT 126:7946

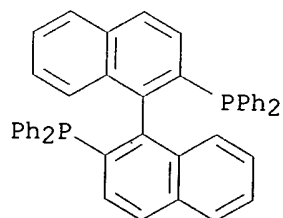
AB The synthesis of oxygen heterocycles was accomplished via a
 palladium-catalyzed intramol. ipso substitution of an aryl halide with an
 alc. The use of chelating bis(phosphine) ligands and a suitable base was
 found to be crucial for achieving good yields of cyclized products. The
 reaction was found to have a reasonable degree of functional group
 compatibility and can be used for the formation of five-, six-, and
 seven-membered oxygen heterocycles. (DPPF)Pd(Br)[2-(2-methyl-2-
 butanol)benzene] [DPPF = 1,1'-bis(diphenylphosphino)ferrocene] was
 isolated, characterized and found to be chem. and kinetically competent as
 an intermediate in the proposed catalytic cycle.

ST palladium catalyst intramol coupling haloarene alc; cyclization aryl
 halide alc; bond formation carbon oxygen

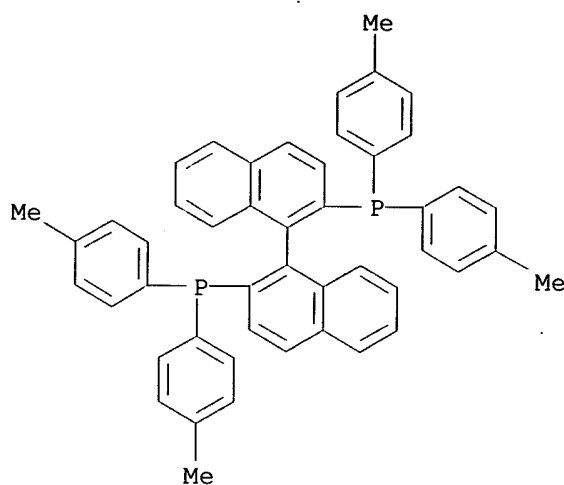
IT Bond formation

(carbon-oxygen; prepn. of oxygen heterocycles by palladium catalyzed
 intramol. coupling of aryl halides with alcs.)

- IT Cross-coupling reaction
Cyclocondensation reaction
(prepn. of oxygen heterocycles by palladium catalyzed intramol.
coupling of aryl halides with alcs.)
- IT Cross-coupling reaction catalysts
RL: CAT (Catalyst use); USES (Uses)
(prepn. of oxygen heterocycles by palladium catalyzed intramol.
coupling of aryl halides with alcs.)
- IT 1198-96-5P 6337-33-3P 13030-26-7P 124773-73-5P 183864-52-0P
183864-53-1P 183864-54-2P 183864-55-3P 183864-56-4P 183864-57-5P
183864-58-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 3375-31-3, Palladium diacetate 7440-05-3, Palladium, uses 12150-46-8,
1,1'-Bis(diphenylphosphino)ferrocene **76189-56-5**,
(S)-(-)-2,2'-Bis(diphenylphosphino)-1,1'-binaphthyl **100165-88-6**
RL: **CAT (Catalyst use)**; USES (Uses)
(prepn. of oxygen heterocycles by palladium catalyzed intramol.
coupling of aryl halides with alcs.)
- IT 67130-96-5 126495-44-1 142569-52-6 183864-38-2 183864-40-6
183864-42-8 183864-44-0 183864-45-1 183864-47-3 183864-49-5
183864-50-8 183864-51-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of oxygen heterocycles by palladium catalyzed intramol.
coupling of aryl halides with alcs.)
- IT 183864-59-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. of oxygen heterocycles by palladium catalyzed intramol.
coupling of aryl halides with alcs.)
- IT **76189-56-5**, (S)-(-)-2,2'-Bis(diphenylphosphino)-1,1'-binaphthyl
100165-88-6
RL: **CAT (Catalyst use)**; USES (Uses)
(prepn. of oxygen heterocycles by palladium catalyzed intramol.
coupling of aryl halides with alcs.)
- RN 76189-56-5 HCAPLUS
- CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA
INDEX NAME)



- RN 100165-88-6 HCAPLUS
- CN Phosphine, (1S)-[1,1'-binaphthalene]-2,2'-diylbis[bis(4-methylphenyl)-
(9CI) (CA INDEX NAME)



- L34 ANSWER 17 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 AN 1996:440836 HCAPLUS
 DN 125:168246
 TI An Improved Procedure for the Resolution of (rac)-
 Ethylenebis(tetrahydroindenyl)Titanium Derivatives
 AU Chin, Bain; **Buchwald, Stephen L.**
 CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge,
 MA, 02139, USA
 SO Journal of Organic Chemistry (1996), 61(16), 5650-5651
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 CC 29-10 (**Organometallic** and **Organometalloidal** Compounds)
 AB The resolu. of (rac)-ethylene-1,2-bis(.eta.5-4,5,6,7-tetrahydro-1-
 indenyl)titanium dichloride [(rac)-1] was effected with
 (R)-2,2'-binaphth-1-ol and p-aminobenzoic acid yielding (S,S)-1 and
 (R,R)-ethylene-1,2-bis(.eta.5-4,5,6,7-tetrahydro-1-indenyl)titanium
 (R)-1,1'-binaphth-2-olate. (S,S)-1 was demonstrated to be an effective
 precatalyst for asym. imine hydrogenation.
 ST resolu ethylenebistetrahydroindenyltitanium dichloride; titanium
 ethylenebistetrahydroindenyl dichloride resolu; imine hydrogenation
 ethylenebistetrahydroindenyltitanium dichloride catalyst
 IT Hydrogenation catalysts
 (ethylenebistetrahydroindenyltitanium compds. for imines)
 IT Resolution
 (of ethylenebistetrahydroindenyltitanium dichloride)
 IT 700-91-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (ethylenebistetrahydroindenyltitanium compds. as catalysts for
 hydrogenation of)
 IT 1006-64-0P, 2-Phenylpyrrolidine
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (ethylenebistetrahydroindenyltitanium compds. as catalysts in prepn.
 of)
 IT 150-13-0, p-Aminobenzoic acid 18531-94-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (in resolu. of ethylenebistetrahydroindenyltitanium dichloride)
 IT 180405-11-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and acidification of)

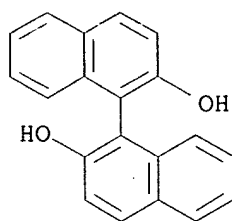
IT 83462-46-8P 143063-72-3P
 RL: CAT (Catalyst use); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (prepn. and hydrogenation catalyst for imines)

IT 83417-94-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (resoln. of)

IT 18531-94-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (in resoln. of ethylenebistetrahydroindenyltitanium dichloride)

RN 18531-94-7 HCAPLUS

CN [1,1'-Binaphthalene]-2,2'-diol, (1R)- (9CI) (CA INDEX NAME)



L34 ANSWER 18 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1996:418146 HCAPLUS

DN 125:167030

TI An Improved Catalyst System for Aromatic Carbon-Nitrogen Bond Formation:
 The Possible Involvement of Bis(Phosphine) Palladium Complexes as Key
 Intermediates

AU **Wolfe, John P.**; Wagaw, Seble; **Buchwald, Stephen L.**

CS Department of Chemistry, Massachusetts Institute of Technology, Cambridge,
 MA, 02139, USA

SO Journal of the American Chemical Society (1996), 118(30),
 7215-7216
 CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

CC 22-4 (Physical Organic Chemistry)

OS CASREACT 125:167030

AB The combination of Pd₂(dba)₃ (dba=dibenzylideneacetone) and BINAP in the
 presence of NaOtBu constitutes a superior catalyst system for the cross
 coupling of amines with aryl bromides. Its success also suggests the
 viability of bis(phosphine)palladium intermediates in the key steps of the
 catalytic cycle. Two complexes, (BINAP)Pd(dba) and (BINAP)Pd(4-t-
 butylphenyl)(Br), were prepd. and were found to be chem. and kinetically
 competent as intermediates in the catalytic sequence.

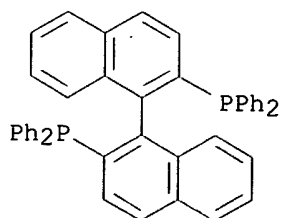
ST arylation amines palladium dba BINAP mechanism

IT Arylation
 Arylation catalysts
 (Pd₂(dba)₃/BINAP in presence of NaOtBu as catalyst for cross-coupling
 of amines with aryl bromides)

IT Aryl bromides
 RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC
 (Process); RACT (Reactant or reagent)
 (Pd₂(dba)₃/BINAP in presence of NaOtBu as catalyst for cross-coupling
 of amines with aryl bromides)

IT Amines, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Pd₂(dba)₃/BINAP in presence of NaOtBu as catalyst for cross-coupling
 of amines with aryl bromides)

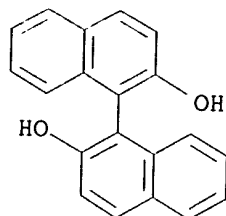
- IT Bond formation
(carbon-nitrogen, Pd2(dba)3/BINAP in presence of NaOtBu as catalyst for cross-coupling of amines with aryl bromides)
- IT 98-06-6
RL: CAT (Catalyst use); FMU (Formation, unclassified); FORM (Formation, nonpreparative); USES (Uses)
(Pd complexes; Pd2(dba)3/BINAP in presence of NaOtBu as catalyst for cross-coupling of amines with aryl bromides)
- IT 6163-58-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(Pd complexes; Pd2(dba)3/BINAP in presence of NaOtBu as catalyst for cross-coupling of amines with aryl bromides)
- IT 51364-51-3, Tris(dibenzylideneacetone)dipalladium 98327-87-8, BINAP
RL: CAT (Catalyst use); USES (Uses)
(Pd2(dba)3/BINAP in presence of NaOtBu as catalyst for cross-coupling of amines with aryl bromides)
- IT 553-94-6, 2-Bromo-p-xylene 556-96-7, 3,5-Dimethylphenyl bromide 578-57-4, 2-Bromoanisole 623-00-7, p-Bromobenzonitrile 698-00-0, 2-Bromo-N,N-dimethylaniline 17789-14-9, 2-(3-Bromophenyl)-1,3-dioxolane 27060-75-9, 4-Bromo-3-methylanisole 69038-74-0, tert-Butyl m-bromobenzoate
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(Pd2(dba)3/BINAP in presence of NaOtBu as catalyst for cross-coupling of amines with aryl bromides)
- IT 100-46-9, Benzylamine, reactions 100-61-8, N-Methylaniline, reactions 108-91-8, Cyclohexylamine, reactions 111-26-2, Hexylamine 2038-03-1, N-(2-Aminoethyl)morpholine
RL: RCT (Reactant); RACT (Reactant or reagent)
(Pd2(dba)3/BINAP in presence of NaOtBu as catalyst for cross-coupling of amines with aryl bromides)
- IT 109-01-3P, N-Methylpiperazine 13342-30-8P 54263-65-9P 124043-95-4P 180336-47-4P 180336-48-5P 180336-49-6P 180336-50-9P 180336-51-0P 180336-52-1P 180336-53-2P 180336-54-3P 180336-55-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Pd2(dba)3/BINAP in presence of NaOtBu as catalyst for cross-coupling of amines with aryl bromides)
- IT 538-58-9
RL: CAT (Catalyst use); FMU (Formation, unclassified); FORM (Formation, nonpreparative); USES (Uses)
(complex with Pd and binap; Pd2(dba)3/BINAP in presence of NaOtBu as catalyst for cross-coupling of amines with aryl bromides)
- IT 98327-87-8, BINAP
RL: CAT (Catalyst use); USES (Uses)
(Pd2(dba)3/BINAP in presence of NaOtBu as catalyst for cross-coupling of amines with aryl bromides)
- RN 98327-87-8 HCAPLUS
- CN Phosphine, [1,1'-binaphthalene]-2,2'-diylbis[diphenyl- (9CI) (CA INDEX NAME)]



- L34 ANSWER 19 OF 19 HCAPLUS COPYRIGHT 2003 ACS
AN 1991:163623 HCAPLUS
DN 114:163623
TI Enantioselective, zirconium-mediated synthesis of allylic amines
AU Grossman, Robert B.; Davis, William M.; Buchwald, Stephen L.
CS Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
SO Journal of the American Chemical Society (1991), 113(6), 2321-2
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 29
OS CASREACT 114:163623
AB The ethylene-1,2-bis(.eta.5-4,5,6,7-tetrahydro-1-indenyl)zirconium dichloride-mediated coupling reaction of a chiral N-arylamines with nonactivated alkynes gave enantiomerically pure allylic N-arylamines. The key step in the reaction sequence is the diastereoselective formation of an imine complex via C-H bond activation. Thus, N-pentylaniline was lithiated and added to (S,S)-ethylene-1,2-bis-.eta.5-4,5,6,7-tetrahydro-1-indenyl)zirconium dichloride trifluoromethanesulfonate and 2-butyne and the intermediate metallacycle complex was hydrolyzed to give 72% (2E,4S)-(+)-4-(phenylamino)-3-methyl-2-octene.
- ST asym synthesis allyl arylamine; alkyne coupling arylamine ethylenebisindenylzirconium chloride; allyl arylamine asym synthesis; anilide coupling alkyne ethylenebisindenylzirconium chloride; arylamine coupling alkyne ethylenebisindenylzirconium chloride; coupling arylamine alkyne ethylenebisindenylzirconium chloride; ethylenebisindenylzirconium chloride coupling arylamine alkyne; pentylanilide coupling butyne ethyleneindenylzirconium chloride; phenylaminomethyloctene asym synthesis; octene phenylaminomethyl asym synthesis; zirconium ethylenebisindenyl coupling arylamine alkyne
- IT Alkynes
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling reaction of, with lithium anilides, chiral ethylenebis(tetrahydroindenyl)zirconium dichloride-catalyzed)
- IT Asymmetric synthesis and induction
(of allylic N-arylamines, by coupling reaction of alkynes with lithium anilides, chiral ethylenebis(tetrahydroindenyl)zirconium dichloride-catalyzed)
- IT Stereochemistry
(of coupling reaction of lithium anilides with alkynes, chiral ethylenebis(tetrahydroindenyl)zirconium dichloride-catalyzed)
- IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aryl, lithiation and coupling reaction of, with alkynes, chiral ethylenebis(tetrahydroindenyl)zirconium dichloride-catalyzed)
- IT Coupling reaction catalysts
(stereoselective, ethylenebis(tetrahydroindenyl)zirconium dichloride, for lithium anilides with alkynes)
- IT Coupling reaction
(stereoselective, of alkynes with lithium anilides, chiral ethylenebis(tetrahydroindenyl)zirconium dichloride-catalyzed)
- IT 20445-33-4, (S)-Methoxytrifluoromethylphenylacetyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with (phenylamino)phenylbutanol)
- IT 18531-99-2, (S)-1,1'-Binaphth-2,2'-diol
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and reaction of, with ethylene bis[tetrahydroindenyl]zirconium dichloride)
- IT 132802-28-9p
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion of, to Mosher ester)
- IT 132802-32-5p

- RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of)
- IT 132802-21-2P, N-[6-(tert-Butyldimethylsilyl)oxy]-1-hexyl]aniline
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and lithiation and reaction of, with
bis(tetrahydroindenyl)dimethylzirconium trifluoromethanesulfonate as
chiral auxiliary and alkyne)
- IT 132881-66-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and methylation of)
- IT 129368-70-3P, 1-Bromo-6-[(tert-butyldimethylsilyl)oxy]hexane
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and reaction of, with aniline)
- IT 132881-67-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and reaction of, with triflic acid, properties of, as chiral
auxiliary for reaction of lithium anilides with alkynes)
- IT 132802-13-2P 132802-14-3P 132802-15-4P 132802-16-5P 132802-17-6P
132802-18-7P 132802-19-8P 132802-20-1P 132802-22-3P 132802-23-4P
132802-24-5P 132802-25-6P 132802-26-7P 132802-27-8P 132802-29-0P
132802-30-3P 132881-68-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 103-32-2, N-Benzylaniline 103-69-5, N-Ethylaniline 104-48-3,
N-Ethyl-p-anisidine 588-47-6, N-Isobutylaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bis(tetrahydroindenyl)dimethylzirconium
trifluoromethanesulfonate as chiral auxiliary and alkynes)
- IT 123-38-6, Propionaldehyde, reactions 592-41-6, 1-Hexene, reactions
673-32-5, 1-Phenyl-1-propyne 6224-91-5, 1-(Trimethylsilyl)-1-propyne
110519-15-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bis(tetrahydroindenyl)dimethylzirconium
trifluoromethanesulfonate as chiral auxiliary and lithium anilide)
- IT 18162-48-6, tert-Butyldimethylchlorosilane
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bromohexanol)
- IT 2655-27-8, N-Pentylaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chiral bis(tetrahydroindenyl)dimethylzirconium
trifluoromethanesulfonate as chiral auxiliary and alkynes)
- IT 503-17-3, 2-Butyne
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chiral bis(tetrahydroindenyl)dimethylzirconium
trifluoromethanesulfonate as chiral auxiliary and lithium anilides)
- IT 100163-29-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chiral lithium binaphthdiol)
- IT 132802-31-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with pentylaniline and butyne)
- IT 4286-55-9, 6-Bromo-1-hexanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(silylation of, with butyldimethylchlorosilane)
- IT 18531-99-2, (S)-1,1'-Binaphth-2,2'-diol
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and reaction of, with ethylene
bis[tetrahydroindenyl]zirconium dichloride)
- RN 18531-99-2 HCAPLUS

CN [1,1'-Binaphthalene]-2,2'-diol, (1S)- (9CI) (CA INDEX NAME)



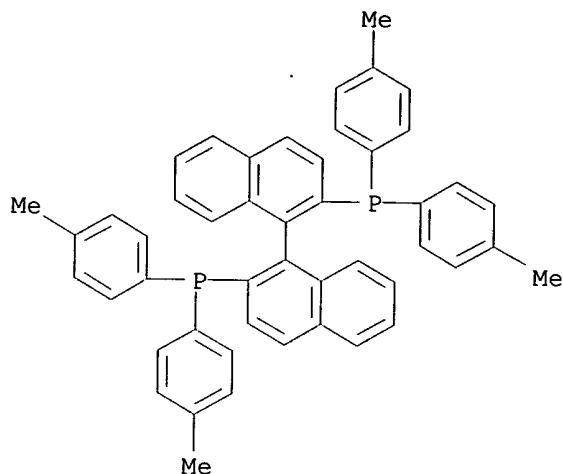
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L35 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2003 ACS
 AN 1998:239186 HCAPLUS
 DN 128:282703
 TI Preparation of aryl ethers
 IN Buchwald, Stephen L.; Wolfe, John P.; Palucki, Michael
 PA Massachusetts Institute of Technology, USA; Buchwald, Stephen L.; Wolfe, John P.; Palucki, Michael
 SO PCT Int. Appl., 72 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM C07C043-20
 ICS C07C041-16; C07C253-30; C07D307-79; C07D311-58; C07D313-08
 CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9815515	A1	19980416	WO 1997-US18719	19971010 <--
	W:			AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM	
	RW:			GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG	
	US 5847166	A	19981208	US 1996-728449	19961010 <--
	AU 9747592	A1	19980505	AU 1997-47592	19971010 <--
	EP 1027316	A1	20000816	EP 1997-910139	19971010 <--
	R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI	
	JP 2001501954	T2	20010213	JP 1998-517804	19971010 <--
	EP 1245553	A2	20021002	EP 2002-12164	19971010 <--
	R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI	
	EP 1254884	A2	20021106	EP 2002-12284	19971010 <--
	R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI	
	US 6166226	A	20001226	US 1998-206820	19981208 <--
	US 2001008942	A1	20010719	US 2000-747280	20001221 <--
PRAI	US 1996-728449	A	19961010		<--
	EP 1997-910139	A3	19971010		<--
	WO 1997-US18719	W	19971010		<--
	US 1998-206820	A1	19981208		<--
OS	CASREACT 128:282703; MARPAT 128:282703				

- AB The title process comprises reaction of an alc. with an arom. compd. ArX in the presence of a base and a transition metal catalyst comprising complexes of Pt, Pd, or Ni such that the activated substituent X conjugate acid HX has a pKa of <5.0. Thus, 2-BrC₆H₄CH₂CMe₂OH was maintained with Pd(OAc)₂ and tol-BINAP in PhMe contg. K₂CO₃ at 100.degree. to give 89% 2,3-dihydro-2,2-dimethylbenzofuran. Kinetic data supporting mechanistic anal. of claimed reactions were given.
- ST aryl ether prepn; alkoxylation aryl halide catalyst
- IT Ethers, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(alkyl aryl; prepn. of aryl ethers)
- IT Etherification catalysts
Etherification kinetics
(prepn. of aryl ethers)
- IT 630-19-3P, Pivalaldehyde
RL: BYP (Byproduct); PREP (Preparation)
(prepn. of aryl ethers)
- IT 193001-13-7P 193001-19-3P 193001-21-7P 193001-31-9P 193001-39-7P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of aryl ethers)
- IT 874-90-8P, 4-Methoxybenzonitrile 1198-96-5P, 3,4-Dihydro-2,2-dimethyl-2H-1-benzopyran 6337-33-3P, 2,2-Dimethyl-2,3-dihydrobenzofuran 13030-26-7P, 3,4-Dihydro-2-methyl-2H-1-benzopyran 21571-62-0P, 1-Cyclohexyloxynaphthalene 24432-40-4P 31603-95-9P 52805-36-4P, 4-Benzyloxybenzonitrile 79615-68-2P, 4-(2,2-Dimethylpropoxy)benzonitrile 91949-95-0P, 4-Isopropoxybenzonitrile 124773-73-5P 183864-52-0P 183864-53-1P 183864-54-2P 183864-55-3P 183864-56-4P 183864-57-5P 185259-36-3P, 4-tert-Butoxybenzonitrile 188527-52-8P 188527-54-0P 188527-60-8P 188527-62-0P 188527-64-2P, 2-Chloro-4-cyclohexyloxybenzonitrile 188527-66-4P, 2-Chloro-4-(1-phenylethoxy)benzonitrile 188527-68-6P, 2-Chloro-4-tert-butoxybenzonitrile 188527-70-0P, 4-Bromo-2-cyclohexyloxybenzonitrile 188527-72-2P, 4-Bromo-2-(1-phenylethoxy)benzonitrile 205752-38-1P, 4-Cyclopentyloxybenzonitrile
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of aryl ethers)
- IT 67-63-0, 2-Propanol, reactions 90-11-9, 1-Bromonaphthalene 96-41-3, Cyclopentanol 98-85-1, 1-Phenylethanol 100-51-6, Benzyl alcohol, reactions 108-93-0, Cyclohexanol, reactions 402-43-7, 4-Bromobenzotrifluoride 584-02-1, 3-Pentanol 623-00-7, 4-Bromobenzonitrile 865-48-5, Sodium tert-butoxide 1564-64-3, 9-Bromoanthracene 2081-44-9 2216-51-5 3972-65-4, 4-tert-Butylbromobenzene 6163-58-2 12150-46-8 51364-51-3 55553-85-0, 1-Propanol, 2,2-Dimethyl-, potassium salt 67130-96-5, 2-Bromo-.alpha.-methylbenzenepropanol 99646-28-3 126495-44-1, 2-Bromo-.alpha.,.alpha.-dimethylbenzeneethanol 142569-52-6 154607-01-9, 4-Bromo-2-chlorobenzonitrile 183864-38-2 183864-40-6 183864-42-8 183864-44-0 183864-45-1 183864-47-3, 2-Bromo-.alpha.,.alpha.-dimethylbenzenepropanol 183864-49-5 183864-50-8 183864-51-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of aryl ethers)
- RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
- RE
- (1) Bates, R; JOURNAL OF ORGANIC CHEMISTRY 1982, V47(22), P4374 HCAPLUS
- (2) Cramer, R; JOURNAL OF ORGANIC CHEMISTRY 1975, V40(16), P2267 HCAPLUS
- IT 99646-28-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of aryl ethers)
- RN 99646-28-3 HCAPLUS

CN Phosphine, (1R)-[1,1'-binaphthalene]-2,2'-diylbis[bis(4-methylphenyl)-
(9CI) (CA INDEX NAME)



L35 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2003 ACS
AN 1994:322918 HCAPLUS
DN 120:322918
TI Catalytic asymmetric and non-asymmetric reduction of imines and oximes
using metal catalysts
IN **Buchwald, Stephen L.**; Willoughby, Christopher A.
PA Massachusetts Institute of Technology, USA
SO U.S., 10 pp. Cont.-in-part of U.S. Ser. No. 698,940, abandoned.
CODEN: USXXAM
DT Patent
LA English
IC ICM C07D207-02
ICS C07D307-02; C07D207-06; C07C209-40; C07C209-52
NCL 548577000
CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 67

FAN.CNT 8

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5292893	A	19940308	US 1991-792229	19911114 <--
	US 5286878	A	19940215	US 1990-616892	19901121 <--
	CA 2096747	AA	19920522	CA 1991-2096747	19911121 <--
	WO 9209545	A2	19920611	WO 1991-US8738	19911121 <--
	WO 9209545	A3	19921029		
	W: CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
	EP 558656	A1	19930908	EP 1992-901632	19911121 <--
	EP 558656	B1	19960417		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 06502867	T2	19940331	JP 1992-502333	19911121 <--
	AT 136878	E	19960515	AT 1992-901632	19911121 <--
	US 5442119	A	19950815	US 1993-90338	19930712 <--
	US 5489682	A	19960206	US 1994-195358	19940210 <--
PRAI	US 1990-616892		19901121	<--	
	US 1991-698940		19910513	<--	
	US 1991-698939		19910513	<--	
	US 1991-749111		19910823	<--	
	US 1991-792227		19911114	<--	
	US 1991-792229		19911114	<--	

US 1991-792233 19911114 <--
WO 1991-US8738 19911121 <--
US 1993-90338 19930712 <--
OS CASREACT 120:322918; MARPAT 120:322918
AB The catalytic asym. redn. of imines [e.g., PhC(:NMe)Me], oximes, and hydrazones using chiral catalysts [e.g., (R,R)-ethylene-1,2-bis(.eta.5-4,5,6,7-tetrahydroindenyl)titanium (R)-1,1'-binaphth-2,2'diolate], to chiral amines (e.g., N-methyl-1-phenylethylamine) is described where the redn. is carried out in the presence of an inert gas or in a H atm., where H is the stoichiometric reducing agent (i.e., hydrogenation).
ST asym redn oxime; imine asym redn prepn amine; catalyst chiral asym hydrogenation imine
IT Imines
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. redn. or hydrogenation of, amines from)
IT Oximes
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. redn. or hydrogenation of, to chiral amines, chiral catalysts for)
IT Siloxanes and Silicones, uses
RL: CAT (Catalyst use); USES (Uses)
(catalysts, contg. chiral transition metal complexes, for asym. hydrogenation or redn. of imines or oximes to chiral amines)
IT Amines, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(chiral, prepn. of, by asym. redn. or hydrogenation of imines or oximes in presence of chiral catalysts)
IT Hydrogenation catalysts
Reduction catalysts
(stereoselective, chiral transition metal complexes, for conversion of imines and oximes to chiral amines)
IT Hydrogenation
Reduction
(stereoselective, of oximes and imines to chiral amines)
IT 700-91-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. hydrogenation of, catalyst for)
IT 6907-71-7, Acetophenone N-methylimine 14428-98-9, Acetophenone N-benzylimine 63459-02-9 143417-07-6 143417-08-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. redn. of, catalyst for)
IT 546-68-9, Titanium tetraisopropoxide 992-92-7, Titanium tetramethoxide 1271-19-8, Titanocene dichloride 3087-36-3, Titanium tetraethoxide 3087-37-4, Titanium tetrapropoxide 3981-83-7, Trichlorotitanium isopropoxide 5593-70-4, Titanium tetrabutoxide 60955-54-6, Titanocene monochloride
RL: CAT (Catalyst use); USES (Uses)
(catalyst, contg. chiral ligands, for asym. hydrogenation or redn. of oximes or imines to chiral amines)
IT 542-91-6, Diethylsilane 693-25-4, n-Pentylmagnesium bromide 775-12-2, Diphenylsilane 998-30-1, Triethoxysilane 1066-26-8, Sodium acetylde 1111-74-6, Dimethylsilane 2487-90-3, Trimethoxysilane 7803-62-5, Silane, uses 22722-98-1, Sodium bis(2-methoxyethoxy)aluminum hydride
RL: CAT (Catalyst use); USES (Uses)
(catalyst, contg. transition metals, for asym. hydrogenation or redn. of oximes or imines to chiral amines)
IT 109-72-8, Butyl lithium, uses 694-53-1, Phenylsilane 83417-93-0 143063-72-3
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for asym. hydrogenation or redn. of oximes or imines to chiral amines)
IT 299-42-3 321-98-2 18531-94-7 18531-99-2 20439-47-8 21436-03-3 93379-49-8

RL: RCT (Reactant); RACT (Reactant or reagent)
 (catalysts contg. transition metals, for asym. hydrogenation or redn.
 of imines or oximes to chiral amines)

IT 1333-74-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrogenation, stereoselective, of oximes and imines to chiral amines)

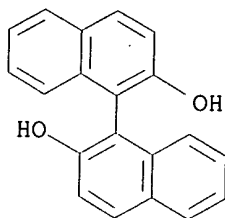
IT 38235-77-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, catalyst for)

IT 1006-64-0P 2084-72-2P 32512-24-6P 61806-77-7P 143063-65-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, enantioselective, catalyst for)

IT 18531-94-7 18531-99-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (catalysts contg. transition metals, for asym. hydrogenation or redn.
 of imines or oximes to chiral amines)

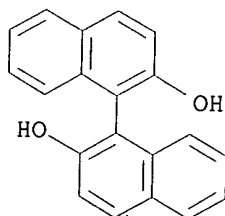
RN 18531-94-7 HCAPLUS

CN [1,1'-Binaphthalene]-2,2'-diol, (1R)- (9CI) (CA INDEX NAME)



RN 18531-99-2 HCAPLUS

CN [1,1'-Binaphthalene]-2,2'-diol, (1S)- (9CI) (CA INDEX NAME)



L35 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2003 ACS

AN 1994:134036 HCAPLUS

DN 120:134036

TI Catalytic asymmetric reduction of acetophenone using metal catalysts

IN **Buchwald, Stephen L.**; Gutierrez, Alberto; Grossman, Robert B.

PA Massachusetts Institute of Technology, USA

SO U.S., 5 pp. Cont.-in-part of U.S. Ser. No. 698,939, abandoned.
 CODEN: USXXAM

DT Patent

LA English

IC ICM C07C029-36
 ICS C07C029-50

NCL 568814000

CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

FAN.CNT 8

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5227538	A	19930713	US 1991-792227	19911114 <--

US 5286878	A	19940215	US 1990-616892	19901121 <--
CA 2096747	AA	19920522	CA 1991-2096747	19911121 <--
WO 9209545	A2	19920611	WO 1991-US8738	19911121 <--
WO 9209545	A3	19921029		

W: CA, JP

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE

EP 558656	A1	19930908	EP 1992-901632	19911121 <--
EP 558656	B1	19960417		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE

JP 06502867	T2	19940331	JP 1992-502333	19911121 <--
AT 136878	E	19960515	AT 1992-901632	19911121 <--

PRAI US 1990-616892 19901121 <--

US 1991-698939 19910513 <--

US 1991-698940 19910513 <--

US 1991-749111 19910823 <--

US 1991-792227 19911114 <--

US 1991-792229 19911114 <--

US 1991-792233 19911114 <--

WO 1991-US8738 19911121 <--

AB A process for the catalytic redn. of the title compd. (I) and in general ketones comprises (i) catalyst M(L)(L')(L''), etc., wherein M = group 3,4,5,6 metal, lanthanide, actinide, L,L',L'' = combination of H, alkyl, aryl, silyl, halo, RO, RS, R'RN wherein R, R' = H, alkyl, aryl; (ii) a stoichiometric amt. of a silane able to supply a hydride ion during the redn. reaction and (iii) a chiral additive such as amine, alc. org. acid, thil and phosphine, reacting a ketone substrate in presence of the mixt., and recovering and purifying the alc. product enriched in one enantiomer. A mixt. of Ti(IV) isopropoxide and triethoxysilane in THF was warmed to 46.degree., (R,R)-1,2-bis(benzylamino)cyclohexane was added followed by I to give MeCHPhOH with an ee of 37% of S enantiomer.

ST acetophenone asym redn catalyst phenylethanol

IT Siloxanes and Silicones, uses

RL: USES (Uses)

(polymethylhydro, reducing agents, for ketones)

IT Ketones, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(redn. of, catalytic)

IT Reduction

(stereoselective, of ketones)

IT Reduction catalysts

(stereoselective, titanium alkoxide, for ketones)

IT 98-86-2, Acetophenone, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(asym. redn. of, catalysts for)

IT 546-68-9, Titanium(IV) isopropoxide

RL: CAT (Catalyst use); USES (Uses)

(catalysts contg., for asym. redn. of acetophenol)

IT 992-92-7, Titanium (IV) methoxide 3087-36-3, Titanium (IV) ethoxide

3981-83-7, Trichlorotitanium (IV) isopropoxide 5593-70-4, Titanium (IV) butoxide

RL: CAT (Catalyst use); USES (Uses)

(catalysts, for asym. redn. of ketones)

IT 93379-48-7 143443-23-6, (R,R)-1,2-Bis(Benzylamino)cyclohexane

RL: RCT (Reactant); RACT (Reactant or reagent)

(chirable additive, in redn. of acetophenone)

IT 299-42-3 321-98-2 18531-94-7 18531-99-2,

(S)-1,1'-Bi-2-naphthol 20439-47-8, (1R,2R)-Diaminocyclohexane

21436-03-3, (1S,2S)-Diaminocyclohexane

RL: RCT (Reactant); RACT (Reactant or reagent)

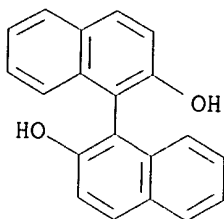
(chiral additive, and redn. of ketones)

IT 98-85-1P, 1-Phenylethanol

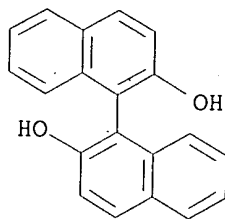
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, by catalytic asym. redn. of acetophenone)

IT 998-30-1, Triethoxysilane
RL: RCT (Reactant); RACT (Reactant or reagent)
(reducing agent, for acetophenone)
IT 18531-94-7 18531-99-2, (S)-1,1'-Bi-2-naphthol
RL: RCT (Reactant); RACT (Reactant or reagent)
(chiral additive, and redn. of ketones)
RN 18531-94-7 HCAPLUS
CN [1,1'-Binaphthalene]-2,2'-diol, (1R)- (9CI) (CA INDEX NAME)



RN 18531-99-2 HCAPLUS
CN [1,1'-Binaphthalene]-2,2'-diol, (1S)- (9CI) (CA INDEX NAME)



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DICTIONARY FILE UPDATES: 11 MAY 2003 HIGHEST RN 514167-89-6

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

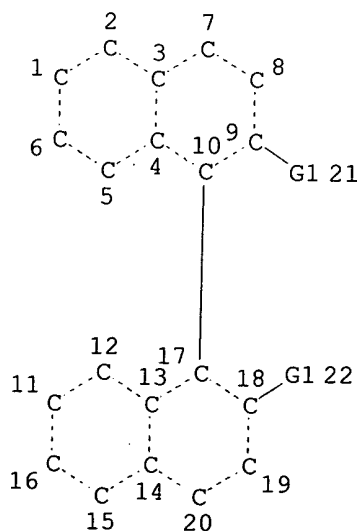
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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L11 3 SEA FILE=REGISTRY ABB=ON PLU=ON L10 AND C34H40NP
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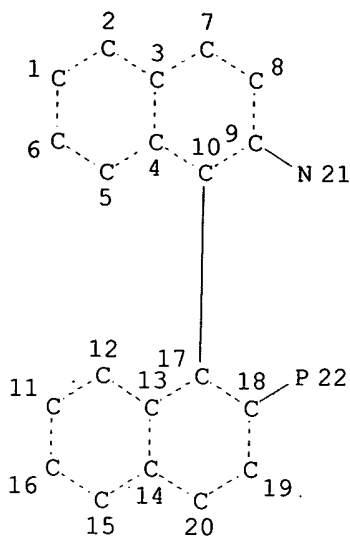
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STEREO ATTRIBUTES: NONE

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L22 6718 SEA FILE=REGISTRY ABB=ON PLU=ON L21 NOT L11

L46 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

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RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L48 75 SEA FILE=REGISTRY SUB=L22 SSS FUL L46

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75 ANSWERS

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FILE 'HCAPLUS' ENTERED AT 09:39:41 ON 12 MAY 2003

L49 30 S L48

L50 7 S L49 AND (PY<=1998 OR PRY<=1998 OR AY<=1998)

L51 5 S L50 NOT L29-L34

L52 2 S L51 AND (PD<=19980710 OR PRD<=19980710 OR AD<=19980710)

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FILE LAST UPDATED: 11 May 2003 (20030511/ED)

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L52 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2003 ACS
AN 1998:787294 HCAPLUS
DN 130:124873
TI Synthesis of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl (MAP) and its accelerating effect on the Pd(0)-catalyzed N-arylation
AU Vyskocil, Stepan; Smrcina, Martin; Kocovsky, Pavel
CS Department of Organic Chemistry, Charles University, Prague, 128 40, Czech Rep.
SO Tetrahedron Letters (1998), 39(50), 9289-9292
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
OS CASREACT 130:124873
AB The title compd., synthesized in four steps from NOBIN, shows a dramatic accelerating effect on the Pd(0)-catalyzed Hartwig-Buchwald N-phenylation of 2'-amino-2-hydroxy-1,1'-binaphthalene and the corresponding diamine with PhBr. Partial kinetic resoln. was obsd. for the phenylation of the racemic amino alc. or diamine in presence of (S)-BINAP.
ST aminodiphenylphosphinobinaphthalene prepn Hartwig Buchwald phenylation catalyst; binaphthylamine phenylation catalyst
IT Arylation
Arylation catalysts
(Hartwig-Buchwald; prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl and its accelerating effect on the Pd(0)-catalyzed N-arylation)
IT 76189-56-5 98327-87-8
RL: CAT (Catalyst use); USES (Uses)
(prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl and its accelerating effect on the Pd(0)-catalyzed N-arylation)
IT 216368-93-3P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl and its accelerating effect on the Pd(0)-catalyzed N-arylation)
IT 108-86-1, Bromobenzene, reactions 4488-22-6, [1,1'-Binaphthalene]-2,2'-diamine 4559-70-0, Diphenylphosphine oxide 18741-85-0 134532-03-9 137848-28-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl and its accelerating effect on the Pd(0)-catalyzed N-arylation)
IT 216320-44-4P 216368-90-0P 216368-92-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl and its accelerating effect on the Pd(0)-catalyzed N-arylation)

IT 17704-02-8P 210094-86-3P 210235-21-5P 216320-20-6P 219820-75-4P
219820-80-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl and its accelerating effect on the Pd(0)-catalyzed N-arylation)

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
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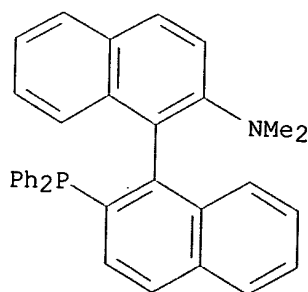
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- (30) Wolfe, J; J Org Chem 1996, V61, P1133 HCAPLUS
- (31) Wolfe, J; J Org Chem 1997, V62, P1264 HCAPLUS

IT 216368-93-3P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)

(prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl and its accelerating effect on the Pd(0)-catalyzed N-arylation)

RN 216368-93-3 HCAPLUS

CN [1,1'-Binaphthalen]-2-amine, 2'-(diphenylphosphino)-N,N-dimethyl-, (1R)-
(9CI) (CA INDEX NAME)

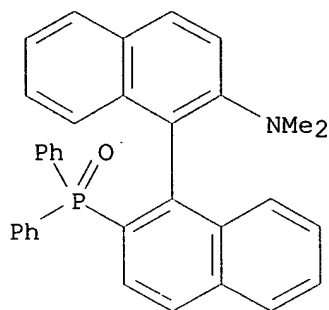
IT 216368-92-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl and its accelerating effect on the Pd(0)-catalyzed N-arylation)

RN 216368-92-2 HCAPLUS

CN [1,1'-Binaphthalen]-2-amine, 2'-(diphenylphosphinyl)-N,N-dimethyl-, (1R)-(9CI) (CA INDEX NAME)



L52 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2003 ACS

AN 1998:659145 HCAPLUS

DN 130:24844

TI Derivatives of 2-Amino-2'-diphenylphosphino-1,1'-binaphthyl (MAP) and Their Application in Asymmetric Palladium(0)-Catalyzed Allylic Substitution

AU Vyskocil, Stepan; Smrcina, Martin; Hanus, Vladimir; Polasek, Miroslav; Kocovsky, Pavel

CS Department of Organic Chemistry, Department of Organic Chemistry Charles University, Prague, Czech Rep.

SO Journal of Organic Chemistry (1998), 63(22), 7738-7748

CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

OS CASREACT 130:24844

AB (R)-(+)-2-Amino-2'-hydroxy-1,1'-binaphthyl (NOBIN) can be readily converted into a series of novel N,N-disubstituted amino phosphines. The N,N-di-Me deriv. (MAP) was prepd. via a sequence involving reductive alkylation with CH₂O and NaBH₄, Pd(0)-catalyzed coupling of the corresponding triflate with Ph₂P(O)H, and redn. of the resulting phosphine oxide with Cl₃SiH. Variation of this scheme was required for the prepn. of other N,N-disubstituted amino phosphines as the phosphinylation failed in the presence of bulky N substituents; the N-protected triflate was first coupled with Ph₂P(O)H, and the resulting phosphine oxide was reduced with Cl₃SiH to give the amino phosphine, which was then subjected to reductive alkylation with individual ketones and NaBH₄. The new P,N-binaphthyls thus obtained (23-25 and 9) were utilized as chiral ligands in Pd(0)-catalyzed allylic substitution. The enantioselectivities obtained for racemic 1,3-diphenylprop-2-en-1-yl acetate and malonate nucleophiles are interpreted in terms of a chelated transition state and preferential attack at the allylic terminus that is trans with respect to the phosphorus acceptor atom.

ST aminodiphenylphosphinobinaphthyl prepn stereoselective allylic substitution catalyst

IT Substitution reaction catalysts

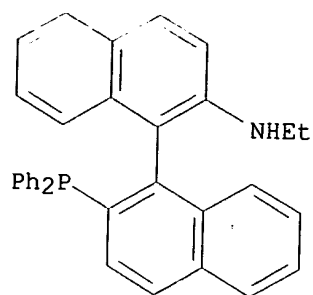
(stereoselective; prepn. of 2-amino-2'-diphenylphosphino-1,1'-

- binaphthyl derivs. as auxiliaries in asym. palladium(0)-catalyzed allylic substitution)
- IT 87802-78-6P 87802-79-7P 216369-05-0P
 RL: BYP (Byproduct); PREP (Preparation)
 (prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as auxiliaries in asym. palladium(0)-catalyzed allylic substitution)
- IT 216368-93-3P 216369-08-3P 216369-09-4P
 216369-10-7P
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as auxiliaries in asym. palladium(0)-catalyzed allylic substitution)
- IT 108-59-8, Dimethyl malonate 609-02-9, Dimethyl methylmalonate
 7217-71-2 21040-45-9, (E)-Cinnamyl acetate 60187-67-9 85217-71-6
 87751-69-7 121440-72-0 137848-28-3 216319-82-3 216319-84-5
 216320-44-4 216368-94-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as auxiliaries in asym. palladium(0)-catalyzed allylic substitution)
- IT 216368-90-0P 216368-92-2P 216369-01-6P 216369-02-7P
 216369-03-8P 216369-04-9P 216369-06-1P
 216369-07-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as auxiliaries in asym. palladium(0)-catalyzed allylic substitution)
- IT 96482-63-2P 96482-64-3P 119793-72-5P 136656-89-8P 189884-53-5P
 216075-90-0P 216319-83-4P 216368-97-7P 216369-00-5P
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 (prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as auxiliaries in asym. palladium(0)-catalyzed allylic substitution)
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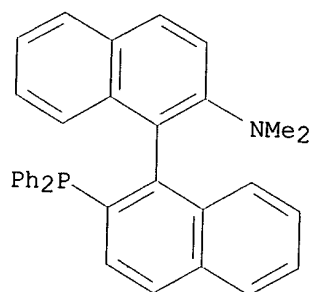
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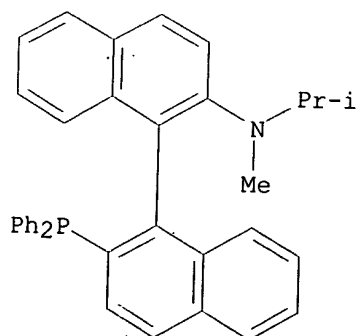
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(CA INDEX NAME)



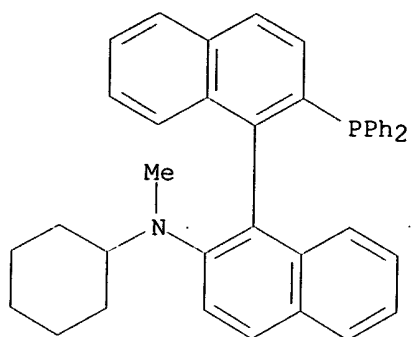
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 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
 USES (Uses)
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 (9CI) (CA INDEX NAME)



RN 216369-08-3 HCAPLUS
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RN 216369-09-4 HCAPLUS
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 , (1R)- (9CI) (CA INDEX NAME)



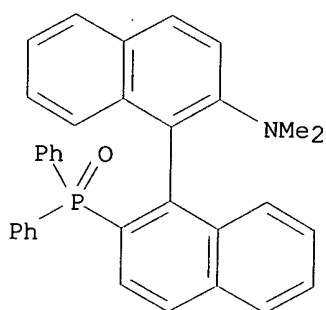
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216369-06-1P 216369-07-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as auxiliaries in asym. palladium(0)-catalyzed allylic substitution)

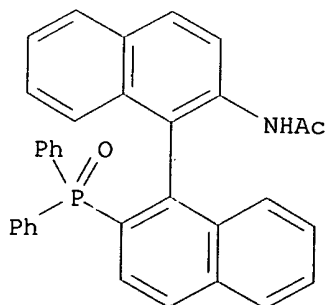
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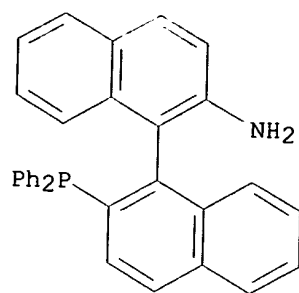
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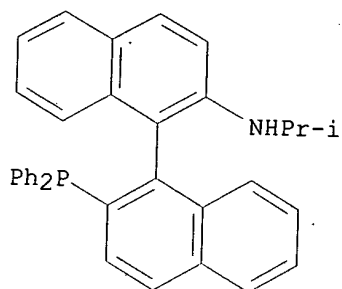


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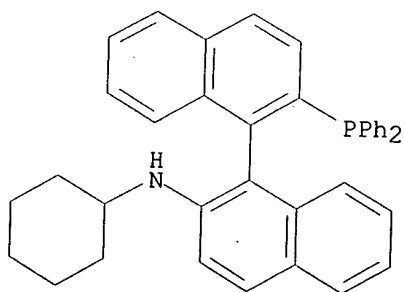
CN [1,1'-Binaphthalen]-2-amine, 2'-(diphenylphosphino)-, (1R)- (9CI) (CA INDEX NAME)



RN 216369-06-1 HCAPLUS
CN [1,1'-Binaphthalen]-2-amine, 2'-(diphenylphosphino)-N-(1-methylethyl)-,
(1R)- (9CI) (CA INDEX NAME)



RN 216369-07-2 HCAPLUS
CN [1,1'-Binaphthalen]-2-amine, N-cyclohexyl-2'-(diphenylphosphino)-, (1R)-
(9CI) (CA INDEX NAME)



=> fil hcaplus

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L81 ANSWER 1 OF 18 HCAPLUS COPYRIGHT 2003 ACS

AN 2000:53646 HCAPLUS

DN 132:108101

TI Biaryl phosphine and amine ligands for improved transition metal-catalyzed processes

IN Buchwald, Stephen; Old, David W.; Wolfe, John P.; Palucki, Michael;
 Kamikawa, Ken; Chieffi, Andrew; Sadighi, Joseph P.; Singer, Robert A.;
 Ahman, Jens

PA Massachusetts Institute of Technology, USA

SO PCT Int. Appl., 397 pp.

CODEN: PIXXD2

DT Patent

LA English

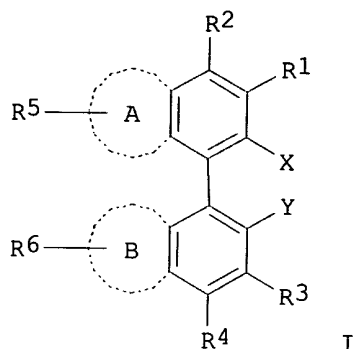
IC ICM C07F009-02

CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 25

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000002887	A2	20000120	WO 1999-US15450	19990709 <--
	WO 2000002887	A3	20000629		
	W: CA, JP				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 6395916	B1	20020528	US 1998-113478	19980710 <--
	US 6307087	B1	20011023	US 1999-231315	19990113 <--
	CA 2336691	AA	20000120	CA 1999-2336691	19990709 <--
	EP 1097158	A2	20010509	EP 1999-933785	19990709 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2002520328	T2	20020709	JP 2000-559117	19990709 <--
PRAI	US 1998-113478	A	19980710	<--	
	US 1998-196855	A	19981120		
	US 1999-231315	A	19990113		
	US 1999-239024	A	19990127		
	WO 1999-US15450	W	19990709		
OS	MARPAT 132:108101				

GI



- AB The present invention relates to the prepn. of novel biaryl phosphine and amine ligands (I) [wherein A and B = independently fused monocyclic or polycyclic cycloalkyl, cycloalkenyl, aryl, or heterocyclic rings of 4-8 atoms; X = NR₂, PR₂, AsR₂, OR, or SR; Y = NR₂, PR₂, AsR₂, OR, SR, SiR₃, alkyl, or H; R-R₆ = independently H, halogen, (hetero)alkyl, alkenyl, alkynyl, hydroxy, alkoxy, silyloxy, amino, nitro, sulfhydryl, amide, carbonyl, ketone, anhydride, silyl, thioalkyl, ketone, ester, nitrile, (hetero)aryl, etc.] for transition metals and their use in metal-catalyzed carbon-heteroatom and carbon-carbon bond-forming reactions. Unexpected improvements over the prior art were demonstrated in transition metal-catalyzed aryl amination reactions, Suzuki couplings giving both biaryl and alkylaryl products, arylations and vinylations at the position .alpha. to carbonyl groups, and carbon-oxygen bond formation. The ligands and methods of the invention enable transformations utilizing aryl chlorides and bromides at room temp. at synthetically useful rates with extremely small amts. of catalyst relative to the limiting reagent. For example, coupling of p-chlorobenzonitrile and morpholine was catalyzed by 2.5 mol% Pd₂(dba)₃, 7.5 mol% of 2-(N,N-dimethylamino)-2'-(dicyclohexylphosphino)biphenyl, and NaOBu-t in DME at room temp. to provide 4-(4-morpholinyl)benzonitrile in 96% yield. Thus, the subject processes provide improvements in many features of the transition metal-catalyzed reactions, including the range of suitable substrates, reaction conditions, and efficiency.
- ST biaryl phosphine ammine ligand prepn transition metal catalyst; amination aryl chloride bromide palladium catalysts; Suzuki coupling aryl chloride bromide palladium catalysts; ketone arylation vinylation palladium catalysts; etherification palladium catalysts
- IT Amines, preparation
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (arom.; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Ethers, preparation
 Ketones, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (arom.; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Aryl halides
 Aryl halides
 RL: RCT (Reactant); RACT (Reactant or reagent)

- (aryl chlorides; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Chlorides, reactions
Chlorides, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aryl; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Transition metal complexes
Transition metal complexes
RL: CAT (Catalyst use); USES (Uses)
(phosphine; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Amination
Amination catalysts
Arylation
Arylation catalysts
Cross-coupling reaction catalysts
Etherification
Etherification catalysts
Suzuki coupling reaction
Vinylolation
Vinylolation catalysts
(prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Phosphines
RL: CAT (Catalyst use); USES (Uses)
(prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Biaryls
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Aryl bromides
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT Phosphines
Phosphines
RL: CAT (Catalyst use); USES (Uses)
(transition metal complexes; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 534-17-8, Dicesium carbonate 3375-31-3, Diacetatopalladium 6476-37-5, Dicyclohexylphenylphosphine 14221-01-3, Tetrakis(triphenylphosphine)palladium 31570-04-4 51364-51-3, Tris(dibenzylideneacetone)dipalladium 54000-83-8, 2,6-Dimethoxyphenyl-di-t-butylphosphine 71042-54-1 74286-11-6 76189-56-5 91548-08-2 100165-88-6 133545-16-1 136779-28-7 139139-92-7 145964-33-6 149341-34-4 155806-35-2 213774-71-1 224311-49-3 247940-06-3 255837-14-0, 2,4,6-Trimethoxyphenyl-di-t-butylphosphine 255837-17-3 255837-19-5 255882-15-6 255882-16-7 255882-17-8 255882-18-9
RL: CAT (Catalyst use); USES (Uses)
(catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations,

- vinylations, and carbon-oxygen bond formation reactions)
- IT 698-00-0P 4688-76-0P 18937-92-3P 20837-12-1P, 2-Bromo-2'-methoxy-1,1'-biphenyl 59734-92-8P 75295-57-7P 89291-23-6P 89787-12-2P, 2-Isopropylphenylboronic acid 128796-39-4P, 4-(Trifluoromethyl)phenylboronic acid 224311-57-3P 224311-58-4P 224311-59-5P 251320-87-3P, 2-Bromo-2'-methylbiphenyl 251320-89-5P, 2-Bromo-2'-isopropylbiphenyl 255837-15-1P, 2-Bromo-4'-(trifluoromethyl)biphenyl 255837-16-2P 255837-18-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 213697-53-1P
 RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (prepd. catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 224311-51-7P, 2-(Di-tert-butylphosphino)biphenyl 224311-52-8P 224311-54-0P 224311-55-1P 251320-85-1P, 2-(Dicyclohexylphosphino)-2'-isopropylbiphenyl 251320-86-2P, 2-(Dicyclohexylphosphino)-2'-methylbiphenyl 255835-81-5P 255835-82-6P 255835-83-7P, 2-(Di-t-butylphosphino)-4'-(trifluoromethyl)biphenyl 255835-84-8P, 2-(Di-t-butylphosphino)-2'-(isopropyl)biphenyl 255835-85-9P 255836-32-9P 255836-65-8P 255836-67-0P 255836-68-1P, 1-[2-(Dicyclohexylphosphino)phenyl]naphthalene 255836-69-2P, 1-[2-(Di-t-butylphosphino)phenyl]naphthalene 255882-14-5P
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (prepd. catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)
- IT 62-53-3, Benzenamine, reactions 75-97-8 88-05-1 88-69-7 90-04-0 91-55-4 93-55-0, Propiophenone 95-65-8 95-68-1 95-72-7 96-22-0, 3-Pentanone 98-54-4 98-80-6 98-86-2, reactions 99-02-5 99-90-1 99-91-2 100-00-5, 1-Chloro-4-nitrobenzene 100-01-6, reactions 100-42-5, reactions 100-46-9, Benzenemethanamine, reactions 100-61-8, reactions 103-69-5 103-88-8, 4'-Bromoacetanilide 104-92-7 104-94-9 105-53-3, Diethyl malonate 106-38-7 106-39-8 106-41-2, 4-Bromophenol 106-43-4 106-49-0, reactions 108-41-8 108-44-1, reactions 108-91-8, Cyclohexanamine, reactions 108-94-1, Cyclohexanone, reactions 109-01-3 109-04-6 109-09-1 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-26-2, 1-Hexanamine 111-92-2 119-61-9, Benzophenone, reactions 120-72-9, Indole, reactions 122-00-9 122-39-4, Diphenylamine, reactions 123-75-1, Pyrrolidine, reactions 141-97-9 280-64-8, 9-BBN 392-83-6, 2-Bromobenzotrifluoride 399-52-0 402-43-7, 4-(Trifluoromethyl)phenyl bromide 460-00-4, 1-Bromo-4-fluorobenzene 502-42-1, Cycloheptanone 504-02-9, 1,3-Cyclohexanedione 529-34-0 530-93-8, .beta.-Tetralone 540-88-5, tert-Butyl acetate 553-94-6 556-96-7 557-93-7, 2-Bromopropene 563-80-4 565-69-5 565-80-0 576-22-7 576-26-1 583-53-9, 1,2-Dibromobenzene 583-55-1, 2-Bromiodobenzene 586-77-6 588-72-7, trans-.beta.-Bromostyrene 590-15-8, trans-1-Bromopropene 591-20-8 592-41-6, 1-Hexene, reactions 615-36-1, 2-Bromoaniline 618-45-1 618-89-3 619-42-1 623-00-7, 4-Bromobenzonitrile 623-03-0 623-12-1 624-31-7 626-55-1, 3-Bromopyridine 626-60-8, 3-Chloropyridine 645-36-3 765-30-0, Cyclopropylamine 766-51-8 766-84-7 778-82-5 782-17-2 872-31-1, 3-Bromothiophene 873-32-5, 2-Chlorobenzonitrile 930-29-0, 1-Chlorocyclopentene 931-51-1, Cyclohexylmagnesium chloride 948-65-2 1003-09-4, 2-Bromothiophene 1013-88-3, Benzophenone imine 1079-66-9, Chlorodiphenylphosphine 1122-91-4, 4-Bromobenzaldehyde 1122-95-8 1126-46-1 1450-65-3 1590-08-5 2038-03-1,

4-Morpholineethanamine 2052-07-5, 2-Bromobiphenyl 2142-68-9,
 2'-Chloroacetophenone 2398-37-0 2635-13-4 2845-89-8 2856-63-5,
 2-Chlorobenzyl cyanide 2905-65-9 3972-65-4, 1-Bromo-4-t-butylbenzene
 4079-52-1 4541-32-6 5350-57-2 5619-07-8, DL-Phenylalanine methyl
 ester hydrochloride 5720-06-9 5798-75-4, Ethyl 4-bromobenzoate
 5892-99-9 6781-98-2 7051-16-3 7073-94-1, 2-Bromoisopropylbenzene
 7524-50-7, L-Phenylalanine methyl ester hydrochloride 7598-28-9
 13716-10-4, Chlorodi-tert-butylphosphine 13922-41-3, 1-Naphthylboronic
 acid 15499-27-1 16081-16-6 16419-60-6 16523-54-9,
 Chlorodicyclohexylphosphine 17496-14-9, 2-Methylindanone 17763-70-1
 17763-80-3 17789-14-9, 2-(3-Bromophenyl)1,3-dioxolane 17933-03-8
 18982-54-2, 2-Bromobenzyl alcohol 22237-13-4, 4-Ethoxyphenylboronic acid
 22867-74-9 24544-04-5 27505-78-8 27752-24-5 36800-95-0,
 4-Cyanophenyl tosylate 40138-16-7, 2-Formylphenylboronic acid
 41085-43-2, 2-Bromo-3-nitrotoluene 41492-05-1 42371-64-2 53847-33-9
 66107-29-7 66107-32-2 74866-28-7, 2,2'-Dibromo-1,1'-binaphthyl
 100379-00-8 100717-47-3 109613-00-5 112042-84-9 154318-75-9
 157282-19-4 158266-43-4 204841-19-0, 3-Acetylphenylboronic acid
 207611-58-3 255837-20-8 255837-21-9 255837-22-0 255837-23-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; prepn. of biaryl phosphine and amine ligands for
 improved palladium-catalyzed amination reactions, Suzuki couplings,
 arylations, vinylations, and carbon-oxygen bond formation reactions)

IT 78235-91-3P 213697-67-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(starting material; prepn. of biaryl phosphine and amine ligands for
 improved palladium-catalyzed amination reactions, Suzuki couplings,
 arylations, vinylations, and carbon-oxygen bond formation reactions)

IT 251320-80-6P, N-(Diphenylmethylene)-2-bromoaniline

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(synthetic product; prepn. of biaryl phosphine and amine ligands for
 improved palladium-catalyzed amination reactions, Suzuki couplings,
 arylations, vinylations, and carbon-oxygen bond formation reactions)

IT 86-26-0P 92-69-3P, 4-Hydroxybiphenyl 92-91-1P, 4-Acetylbiphenyl
 92-93-3P, 4-Nitrobiphenyl 101-70-2P, 4,4'-Dimethoxydiphenylamine
 121-00-6P 613-37-6P, 4-Methoxybiphenyl 620-83-7P 620-93-9P,
 Di-p-tolylamine 644-08-6P, 4-Methylbiphenyl 720-75-2P, Methyl
 4-phenylbenzoate 730-11-0P, 4-Methoxy-4'-nitrodiphenylamine 774-52-7P,
 N-(4-Methylphenyl)piperidine 825-54-7P 825-55-8P, 2-Phenylthiophene
 1208-86-2P 1625-92-9P, 4-t-Butylbiphenyl 2142-66-7P, 2-Acetylbiphenyl
 2920-38-9P, 4-Cyanobiphenyl 2928-43-0P, 2-(Hydroxymethyl)biphenyl
 3077-16-5P, N-(4-Methylphenyl)morpholine 3470-65-3P 3976-34-9P,
 2,6-Dimethylbiphenyl 4036-43-5P 4075-79-0P, N-Acetyl-4-aminobiphenyl
 4316-51-2P, N-(4-Methoxyphenyl)-N,N-diphenylamine 4316-53-4P
 4496-49-5P 4787-76-2P, N-(2-Methoxyphenyl)pyrrolidine 5031-78-7P
 5405-15-2P, N-Benzyl-p-toluidine 5405-19-6P 6574-15-8P,
 N-(4-Nitrophenyl)piperidine 6935-27-9P, N-Benzyl-2-aminopyridine
 7372-85-2P, 2,5-Dimethylbiphenyl 10273-87-7P 10282-31-2P,
 N-(4-Cyanophenyl)morpholine 15359-99-6P 15360-00-6P 16251-99-3P
 16819-50-4P, N-(2,6-Dimethylphenyl)benzylamine 17057-88-4P,
 3,5-Dimethylbiphenyl 17952-07-7P 19853-10-2P, [1,1'-Biphenyl]-2-
 acetonitrile 21218-94-0P 23600-89-7P 23676-05-3P 23699-65-2P,
 N-(3-Acetylphenyl)aniline 23951-29-3P 24255-25-2P,
 N-(2-Pyridyl)morpholine 25539-14-4P 25699-92-7P, N-(4-
 Cyanophenyl)indole 25700-23-6P, N-(3-Pyridyl)indole 27347-14-4P
 31144-33-9P 31603-95-9P, 4-tert-Butyl-1-tert-butyloxybenzene
 34160-16-2P 35393-20-5P, N-(Diphenylmethylene)-4-nitroaniline
 38158-65-5P 38869-05-5P 39253-43-5P 39910-98-0P,
 N-(4-Acetylphenyl)morpholine 50798-94-2P, N-(2-Methoxyphenyl)benzylamine
 50910-08-2P, N-(2-Pyridyl)-N,N-diphenylamine 51580-77-9P 51786-49-3P
 52351-44-7P, N-(4-Methoxyphenyl)-2-phenylindole 54480-44-3P,

4-Methoxy-4'-(dimethylamino)diphenylamine 54660-04-7P,
N-(4-Methoxyphenyl)pyrrolidine 55251-46-2P 56052-33-6P 56506-60-6P,
N-(4-Methylphenyl)hexylamine 56915-80-1P, 1-(3-Acetylphenyl)-4-
methylpiperazine 60893-66-5P 61394-81-8P 62787-14-8P 62787-15-9P
62790-83-4P 62790-85-6P 68856-26-8P 70945-85-6P 75201-55-7P
75934-30-4P 76650-29-8P, 4-Acetyl-3'-methylbiphenyl 76708-72-0P
76708-78-6P, 2,5,3'-Trimethylbiphenyl 77422-28-7P 81693-80-3P,
4-Hexylanisole 82749-62-0P 83188-35-6P 84736-47-0P,
N-(4-t-Butylphenyl)morpholine 84736-54-9P, 2-(4-Methoxyphenyl)-3-
pentanone 84839-92-9P 84839-93-0P 91949-95-0P, 4-
Isopropoxybenzonitrile 92495-53-9P, 4-Methyl-2'-methoxybiphenyl
92670-29-6P, N-(3-Pyridyl)morpholine 93597-01-4P, N-(4-
Methoxyphenyl)indole 94540-42-8P 94959-58-7P 97053-04-8P
97413-60-0P 114081-08-2P 114772-53-1P 116267-90-4P,
N-(3-Thiophenyl)-N,N-diphenylamine 123324-87-8P 124043-95-4P
129644-26-4P 137445-01-3P 138900-16-0P, N-(4-Fluorophenyl)indole
138900-19-3P 146803-96-5P 167283-32-1P, N-(4-Methylphenyl)indole
171092-38-9P, 3-(3-Acetylphenyl)pyridine 172878-95-4P 174307-96-1P
175696-73-8P, N-(3-Cyanophenyl)pyrrolidine 179487-70-8P 180336-54-3P,
N-(2,5-Dimethylphenyl)-N-methylaniline 183135-51-5P,
N-Methyl-N-(3-pyridyl)aniline 183135-52-6P 185259-34-1P,
N-(4-t-Butylphenyl)piperidine 188026-55-3P, N,N-Dibutyl-4-t-butylaniline
188026-64-4P, N-Ethyl-N-(3,5-dimethylphenyl)aniline 188026-74-6P
196604-19-0P 196604-21-4P 196604-24-7P 197172-67-1P 197172-69-3P
197640-99-6P 202802-70-8P 211292-60-3P 211292-66-9P,
2,6-Diisopropyl-2',6'-dimethyldiphenylamine 212382-74-6P 213014-13-2P
213697-51-9P 213697-52-0P, 2,6-Dimethyl-N-hexylaniline 213697-65-5P,
1,1-Bis(4-methylphenyl)-3-methyl-2-butanone 213697-66-6P 215394-88-0P
223248-27-9P 223655-23-0P 224311-62-0P 224311-63-1P 224311-65-3P
224311-66-4P 224311-67-5P 224311-68-6P 224311-69-7P 224311-70-0P
224311-72-2P 224311-73-3P 224311-74-4P 224311-75-5P 224311-76-6P
226569-78-4P 226917-75-5P, N-(4-Cyanophenyl)hexylamine 247940-07-4P,
N-Methyl-N-(3,5-dimethoxyphenyl)aniline 247940-08-5P 251320-76-0P
251320-77-1P, 4-Formyl-4'-ethoxybiphenyl 251320-78-2P 251320-79-3P
251320-81-7P, 3-Acetyl-3',5'-dimethoxybiphenyl 251320-82-8P
251320-83-9P 251320-84-0P, 2-Methoxy-2'-acetylbiiphenyl 253768-96-6P,
N-(3-Cyanophenyl)benzylamine 255835-86-0P 255835-87-1P 255835-88-2P
255835-89-3P 255835-90-6P 255835-91-7P, N-(2,6-
Dimethylphenyl)morpholine 255835-92-8P 255835-93-9P,
N-(4-t-Butylphenyl)benzylamine 255835-94-0P, N-(3,4-
Dimethylphenyl)pyrrolidine 255835-95-1P, 2-Methoxy-4'-cyanodiphenylamine
255835-96-2P 255835-97-3P 255835-98-4P 255835-99-5P 255836-00-1P
255836-01-2P 255836-02-3P 255836-04-5P, N-(2-Methoxyphenyl)-N-(3-
methoxyphenyl)-N-(4-methoxyphenyl)amine 255836-06-7P,
N-(4-Dimethylaminophenyl)-N-(4-methoxyphenyl)-N-(3-methylphenyl)amine
255836-08-9P, N-(2,4-Dimethylphenyl)-N-(4-methoxyphenyl)-N-(3-
methylphenyl)amine 255836-10-3P 255836-12-5P 255836-14-7P,
N-(4-Butylphenyl)-N-(4-methoxyphenyl)-N-(4-methylphenyl)amine
255836-15-8P, N-(2,5-Dimethylphenyl)-N-(3,5-dimethylphenyl)-N-(4-
methylphenyl)amine 255836-17-0P 255836-19-2P, N-(4-tert-
Butylphenyl)indole 255836-21-6P 255836-23-8P, N-Cyclopropyl-4-tert-
butylaniline 255836-25-0P, N-Cyclopropyl-2,5-dimethylaniline
255836-28-3P 255836-30-7P 255836-36-3P 255836-38-5P 255836-39-6P
255836-41-0P 255836-43-2P 255836-44-3P 255836-45-4P,
2-Methyl-4-(4-butylphenyl)-3-pentanone 255836-46-5P 255836-48-7P
255836-50-1P 255836-52-3P 255836-54-5P, 2-(3-Hydroxyphenyl)-3-
pentanone 255836-56-7P, 2,4-Dimethyl-2-(4-t-butylphenyl)-3-pentanone
255836-57-8P 255836-59-0P 255836-61-4P 255836-63-6P 255836-70-5P,
N-(4-t-Butylphenyl)-2-phenylindole 255836-72-7P 255836-74-9P,
N-(3,5-Dimethylphenyl)-2,3-dimethylindole 255836-76-1P,
N-(4-t-Butylphenyl)-2,3,7-trimethylindole 255836-78-3P 255836-80-7P,
N-(2-Pyridyl)-7-ethylindole 255836-82-9P, N-(3,5-Dimethylphenyl)-7-
ethylindole 255836-84-1P 255836-86-3P 255836-88-5P 255836-90-9P

255836-92-1P 255836-94-3P 255836-95-4P 255836-96-5P 255836-97-6P
 255836-98-7P 255836-99-8P 255837-00-4P 255837-01-5P 255837-02-6P
 255837-03-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthetic product; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT 255837-04-8P 255837-05-9P 255837-06-0P 255837-07-1P 255837-08-2P
 255837-09-3P 255837-10-6P 255837-11-7P 255837-12-8P 255837-13-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthetic product; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

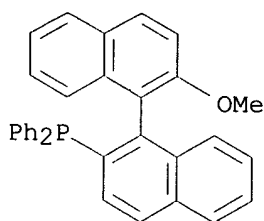
IT 145964-33-6

RL: CAT (Catalyst use); USES (Uses)

(catalyst; prepn. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

RN 145964-33-6 HCAPLUS

CN Phosphine, [(1R)-2'-methoxy[1,1'-binaphthalen]-2-yl]diphenyl- (9CI) (CA INDEX NAME)



L81 ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2003 ACS

AN 1998:618676 HCAPLUS

DN 129:245667

TI Optically active phosphine derivative having at least two vinyl groups, polymer produced using the same as monomer and transition metal complexes of these

IN Tamao, Kyoko; Itoi, Yohei

PA Takasago International Corp., Japan

SO Eur. Pat. Appl., 26 pp.

CODEN: EPXXDW

DT Patent

LA English

IC ICM C07F009-6574

ICS C07F015-00; C08F030-02; C08F030-04; C07C045-50; C07B053-00

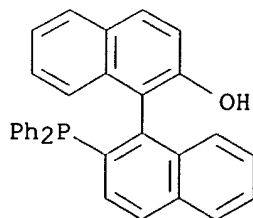
ICI C07M007-00

CC 35-3 (Chemistry of Synthetic High Polymers)

FAN.CNT 1

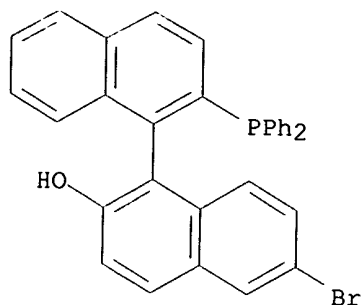
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 864577	A2	19980916	EP 1998-301763	19980310 <--
	EP 864577	A3	19990825		
	EP 864577	B1	20030205		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 10251282	A2	19980922	JP 1997-72817	19970311 <--
	US 6143834	A	20001107	US 1998-38280	19980311 <--
	US 6248848	B1	20010619	US 2000-603991	20000627 <--
PRAI	JP 1997-72817	A	19970311	<--	
	US 1998-38280	A3	19980311	<--	

- OS MARPAT 129:245667
- AB Specified 2'-diarylphosphino-1,1'-biphenylen-2-yloxy(6,6'-divinyl-1,1'-binaphthalene -2,2'-diyloxy)phosphine derivs. are useful in polymers and transition metal complexes. Also disclosed are a polymer having structural units derived from the phosphine deriv. and a transition metal complex obtained by causing a transition metal compd. to act on the phosphine deriv. or the polymer. A novel polymer-supported ligand is provided which, when used as a catalyst for asym. syntheses, gives satisfactory results concerning catalytic activity, enantiomer excess, etc.
- ST optically active phosphine deriv polymer; transition metal complex phosphine polymer
- IT Hydroformylation catalysts
(optically active phosphine deriv. having at least two vinyl groups, polymer produced using the same as monomer and transition metal complexes of these)
- IT 100-42-5DP, hydroformylated 14874-82-9DP, Rhodium dicarbonylacetylacetonate, complexes with 2'-diarylphosphino-1,1'-biphenylen-2-yloxy(6,6'-divinyl-1,1'-binaphthalene -2,2'-diyloxy)phosphine polymers 213188-62-6P 213188-64-8P
RL: IMF (Industrial manufacture); PREP (Preparation)
(optically active phosphine deriv. having at least two vinyl groups, polymer produced using the same as monomer and transition metal complexes of these)
- IT 80655-81-8P 126613-06-7P 132532-04-8P 132548-91-5P
149917-88-4P 187742-81-0P 205238-73-9P 205238-75-1P
213314-12-6P 213314-13-7P 213314-14-8P 213314-15-9P 213314-16-0P
213314-17-1P 213314-18-2P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(optically active phosphine deriv. having at least two vinyl groups, polymer produced using the same as monomer and transition metal complexes of these)
- IT 68-12-2, Dimethylformamide, reactions 358-23-6, Trifluoromethanesulfonic anhydride 6737-42-4, 1,3-Bis(diphenylphosphino)propane 7726-95-6, Bromine, reactions 18531-94-7 18531-99-2 69739-34-0, Tert-Butyldimethylsilyltriflate
RL: RCT (Reactant); RACT (Reactant or reagent)
(optically active phosphine deriv. having at least two vinyl groups, polymer produced using the same as monomer and transition metal complexes of these)
- IT **149917-88-4P 213314-17-1P 213314-18-2P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(optically active phosphine deriv. having at least two vinyl groups, polymer produced using the same as monomer and transition metal complexes of these)
- RN 149917-88-4 HCAPLUS
- CN [1,1'-Binaphthalen]-2-ol, 2'-(diphenylphosphino)-, (1R)- (9CI) (CA INDEX NAME)



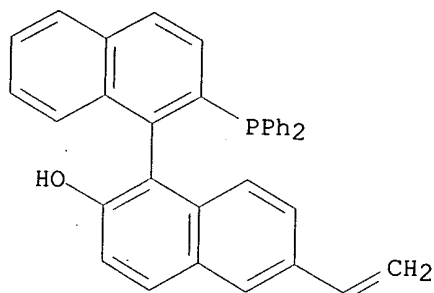
RN 213314-17-1 HCAPLUS

CN [1,1'-Binaphthalen]-2-ol, 6-bromo-2'-(diphenylphosphino)-, (1R)- (9CI)
(CA INDEX NAME)



RN 213314-18-2 HCAPLUS

CN [1,1'-Binaphthalen]-2-ol, 2'-(diphenylphosphino)-6-ethenyl-, (1R)- (9CI)
(CA INDEX NAME)



L81 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2003 ACS

AN 1998:614290 HCAPLUS

DN 129:316694

TI Preparation of vinyl-containing chiral phosphines, their polymers, and their transition metal complexes as catalysts for asymmetric hydroformylation

IN Tamao, Kyoko; Itoi, Yohei

PA Takasago Perfumery Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DT **Patent**

LA Japanese

IC ICM C07F009-6574

ICS B01J031-24; C07F015-00; C08F012-32; C08F212-04; C08F212-36

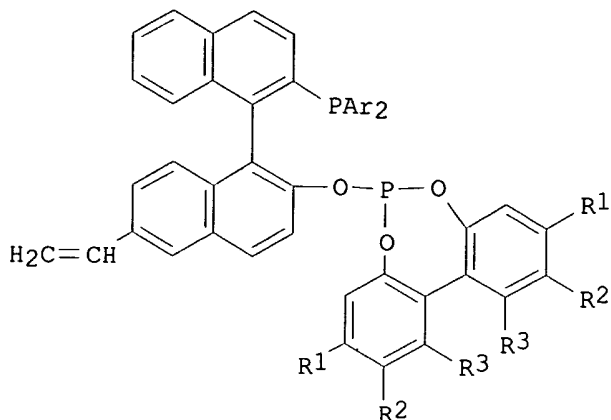
CC 35-2 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 29, 38, 67

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10251283	A2	19980922	JP 1997-72838	19970311 <--
	EP 877029	A2	19981111	EP 1998-301768	19980310 <--
	EP 877029	A3	19990825		
	EP 877029	B1	20021211		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	US 6022936	A	20000208	US 1998-38131	19980311 <--
PRAI	JP 1997-72838	A	19970311	<--	

OS MARPAT 129:316694
GI



I

- AB Title phosphines I [Ar = (substituted) Ph, (substituted) naphthyl; R1, R2 = H, lower (halo)alkyl, lower alkoxy, halo, benzyloxy; R3 = lower (halo)alkyl, lower alkoxy, halo, benzyloxy; R2, R3 may form hydrocarbon ring], their transition metal complexes, polymers or oligomers prep'd. by soln. or suspension polymn. of I, and transition metal complexes of the polymers or oligomers are prep'd. Optically active R5CHMeCHO [R5 = C1-8 alkyl, (substituted) Ph, naphthyl, acetoxy, etc.] are prep'd. by asym. hydroformylation of R5CH:CH2 (R5 = same as above) using the polymer transition metal complexes. Condensation of (R)-2'-diphenylphosphino-2-hydroxy-6-vinyl-1,1'-binaphthyl (prepn. given) with (S)-1,1'-binaphthalene-2,2'-dioxychlorophosphine in ether in the presence of Et3N at room temp. for 24 h gave 69% optically active I (Ar = Ph, R1 = H, R2-R3 = CH:CHCH:CH), which was polym'd. with styrene and divinylbenzene and treated with Rh(acac)(CO)2 to give a complex. Styrene was hydroformylated by CO and H in C6H6 using the complex at 60.degree. under 50 atm for 40 h to give PhCHMeCHO with 94% selectivity and 82% ee optical purity at 97% conversion.
- ST chiral phosphine polymer complex catalyst; styrene asym hydroformylation catalyst phosphine polymer; aldehyde prep'n asym hydroformylation olefin; transition metal complex phosphine polymer catalyst; vinyl binaphthylphosphine polymer complex catalyst
- IT Hydroformylation catalysts
(asym.; prep'n. of vinyl-contg. chiral phosphines for polymeric transition metal complexes as catalysts for asym. hydroformylation)
- IT Aldehydes, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(chiral; prep'n. of vinyl-contg. chiral phosphines for polymeric transition metal complexes as catalysts for asym. hydroformylation)
- IT Transition metal complexes
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(phosphine; prep'n. of vinyl-contg. chiral phosphines for polymeric transition metal complexes as catalysts for asym. hydroformylation)
- IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(prep'n. of vinyl-contg. chiral phosphines for polymeric transition metal complexes as catalysts for asym. hydroformylation)
- IT Phosphines

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)

(transition metal complexes; prepn. of vinyl-contg. chiral phosphines
for polymeric transition metal complexes as catalysts for asym.
hydroformylation)

IT 7440-16-6DP, Rhodium, complexes with chiral phosphine-contg. polymer,
preparation 205238-71-7DP, rhodium complex
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)

(prepn. of vinyl-contg. chiral phosphines for polymeric transition
metal complexes as catalysts for asym. hydroformylation)

IT 93-53-8P, .alpha.-Methylphenylacetaldehyde
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)

(prepn. of vinyl-contg. chiral phosphines for polymeric transition
metal complexes as catalysts for asym. hydroformylation)

IT 100-42-5, reactions 4559-70-0, Diphenylphosphine oxide 18531-94-7
137156-22-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of vinyl-contg. chiral phosphines for polymeric transition
metal complexes as catalysts for asym. hydroformylation)

IT 126613-06-7P 132532-04-8P 132548-91-5P 205238-71-7P 213314-16-0P
213314-17-1P 213314-18-2P 214913-51-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(prepn. of vinyl-contg. chiral phosphines for polymeric transition
metal complexes as catalysts for asym. hydroformylation)

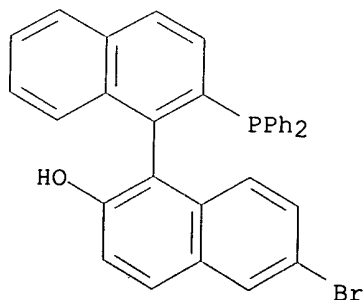
IT 213314-17-1P 213314-18-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(prepn. of vinyl-contg. chiral phosphines for polymeric transition
metal complexes as catalysts for asym. hydroformylation)

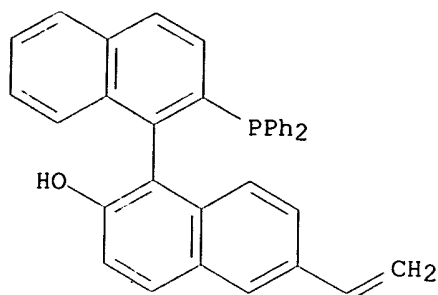
RN 213314-17-1 HCAPLUS

CN [1,1'-Binaphthalen]-2-ol, 6-bromo-2'-(diphenylphosphino)-, (1R)- (9CI)
(CA INDEX NAME)



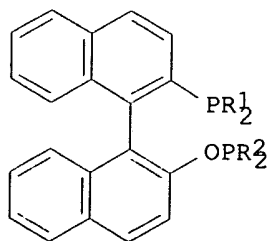
RN 213314-18-2 HCAPLUS

CN [1,1'-Binaphthalen]-2-ol, 2'-(diphenylphosphino)-6-ethenyl-, (1R)- (9CI)
(CA INDEX NAME)

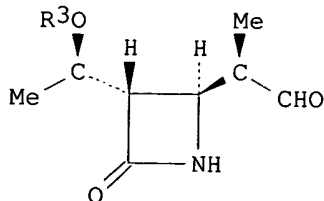


L81 ANSWER 4 OF 18 HCAPLUS COPYRIGHT 2003 ACS
 AN 1997:195644 HCAPLUS
 DN 126:186205
 TI Preparation of chiral binaphthalene phosphine-phosphinite compounds and their use in asymmetric synthesis of 4-[(R)-1'-formylethyl]azetidin-2-one derivatives by hydroformylation
 IN Saito, Takao; Matsumura, Kazuhiko; Miura, Takashi; Kumobayashi, Hidenori; Yoshida, Akifumi
 PA Takasago International Corporation, Japan
 SO Eur. Pat. Appl., 26 pp.
 CODEN: EPXXDW
 DT **Patent**
 LA English
 IC ICM C07F009-46
 ICS C07D205-08
 CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 22, 27, 67
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 755937	A1	19970129	EP 1996-305182	19960715 <--
	EP 755937	B1	20021023		
	R: CH, DE, FR, GB, IT, LI, NL				
	JP 09040684	A2	19970210	JP 1995-210215	19950727 <--
	US 5824822	A	19981020	US 1996-677226	19960709 <--
PRAI	JP 1995-210215	A	19950727 <--		
OS	CASREACT 126:186205; MARPAT 126:186205				
GI					



I



II

AB Phosphine-phosphinite compds. (R)-I (R1, R2 = substituted or unsubstituted Ph, naphthyl) and a process for prepg. a 4-[(R)-1'-formylethyl]azetidin-2-one deriv. II (R3 = H, protective group for a hydroxyl group) using (R)-I are claimed. (R)-I, either in combination, or as a complex, with a transition metal compd., is useful as a catalyst for asym. hydroformylation and makes it possible to easily synthesize an important

intermediate for carbapenem antibiotics or a precursor thereof at high regioselectivity and diastereoselectivity. For example, (3S,4R)-3-((R)-1-tert-butyldimethylsilyloxy)ethyl-4-((R)-1'-formylethyl)azetidin-2-one, (3S,4R)-3-((R)-1-tert-butyldimethylsilyloxy)ethyl-4-((S)-1'-formylethyl)azetidin-2-one, and (3S,4R)-3-((R)-1-tert-butyldimethylsilyloxy)ethyl-4-(2-formylethyl)azetidin-2-one were formed in 68.4/3.6/28 ratio and, after chromatog., a 68% yield of the 1st 2 compds. with 95/5 isomer ratio was obtained in the presence of (R)-I (R1 = 3,5-dimethylphenyl; R2 = Ph) and [Rh(COD)Cl]₂; other phosphine-phosphinite compds. such as (R)-I (R1 = Ph; R2 = OPh) gave significantly inferior results. The detailed prepn. of (R)-I (R1 = 3,5-dimethylphenyl; R2 = Ph) is given and results of catalytic tests are given for about 20 (R)-I.

- ST binaphthyl phosphine phosphinite metal hydroformylation catalyst; vinylazetidinone asym hydroformylation catalyst; formylethylazetidinone asym synthesis hydroformylation catalyst; azetidinone formylethyl asym synthesis; chiral binaphthalene phosphine phosphinite hydroformylation catalyst
- IT Hydroformylation catalysts
(asym., regioselective; binaphthyl phosphine-phosphinite compds. in combination or as complex with transition metal compd. for vinylazetidinone)
- IT Asymmetric synthesis and induction
(of (formylethyl)azetidinone in presence of binaphthyl phosphine-phosphinite compds. in combination or as complex with transition metal compd.)
- IT Regiochemistry
Stereochemistry
(of hydroformylation of vinylazetidinone in presence of binaphthyl phosphine-phosphinite compds. in combination or as complex with transition metal compd.)
- IT 112256-72-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. hydroformylation in presence of binaphthalene phosphine-phosphinite compds. in combination or as complex with transition metal compd.)
- IT 159496-98-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis in presence of binaphthalene phosphine-phosphinite compds. in combination or as complex with transition metal compd.)
- IT 12092-47-6, Bis(chloro(1,5-cyclooctadiene)rhodium) 14874-82-9, (Acetylacetonato)dicarbonylrhodium
RL: CAT (Catalyst use); USES (Uses)
(asym. synthesis of (formylethyl)azetidinone in presence of binaphthalene phosphine-phosphinite compds. in combination or as complex with transition metal compd.)
- IT 183119-22-4P 183119-23-5P 183119-24-6P 187461-34-3P 187461-37-6P
187461-39-8P 187461-41-2P 187461-43-4P 187461-44-5P 187461-45-6P
187461-46-7P 187461-47-8P 187461-48-9P 187461-49-0P 187461-50-3P
187461-51-4P 187461-52-5P 187461-53-6P 187461-54-7P
187461-55-8P 187461-56-9P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(binaphthalene phosphine-phosphinite compd. in combination or as complex with transition metal compd. for asym. synthesis of (formylethyl)azetidinone)
- IT 358-23-6, Trifluoromethanesulfonic anhydride 556-96-7, 5-Bromo-m-xylene 762-04-9, Diethyl phosphite 1019-71-2, Chlorobis(4-methylphenyl)phosphine 1079-66-9, Chlorodiphenylphosphine 4559-70-0, Diphenylphosphine oxide 13685-24-0, Chlorobis(4-(trifluoromethyl)phenyl)phosphine 18531-94-7, (R)-1,1'-Bi-2-naphthol 23039-97-6, Chlorobis(4-fluorophenyl)phosphine 30309-80-9, Bis(o-tolyl)phosphine oxide 74289-57-9, Chlorobis(3,5-

dimethylphenyl)phosphine 78871-05-3, Bis(2-naphthyl)phosphine oxide 142421-57-6, Bis(3,5-bis(trifluoromethyl)phenyl)(chloro)phosphine 159418-72-1, Chlorobis(3,5-difluorophenyl)phosphine 187344-92-9, Bis(3,5-dimethylphenyl)phosphine oxide 187344-93-0, Bis(6-methoxy-2-naphthyl)phosphine oxide 187344-94-1, Bis(3-biphenyl)phosphine oxide 187344-95-2, Bis(4-biphenyl)phosphine oxide 187344-96-3, Bis(4-(2,4,6-trimethylphenyl)phenyl)phosphine oxide 187344-97-4, Dicyclopentylphosphine oxide 187344-98-5, Bis(3,5-bis(trimethylsilyl)phenyl)phosphine oxide 187344-99-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(for prepn. of binaphthalene phosphine-phosphinite compd. for asym. hydroformylation catalysis)

IT 126613-06-7P, (R)-2,2'-Bis(trifluoromethanesulfonyloxy)-1,1'-binaphthalene **149917-89-5P** 187461-57-0P 187461-58-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for prepn. of binaphthalene phosphine-phosphinite compd. for asym. hydroformylation catalysis)

IT 183119-15-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

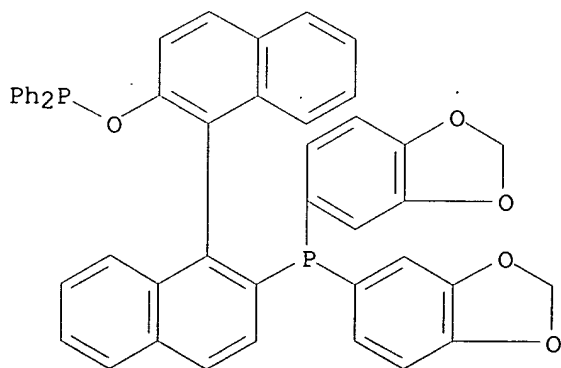
IT **187461-55-8P**

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(binaphthalene phosphine-phosphinite compd. in combination or as complex with transition metal compd. for asym. synthesis of (formylethyl)azetidinone)

RN 187461-55-8 HCAPLUS

CN Phosphinous acid, diphenyl-, 2'-[bis(1,3-benzodioxol-5-yl)phosphino][1,1'-binaphthalen]-2-yl ester, (R)- (9CI) (CA INDEX NAME)



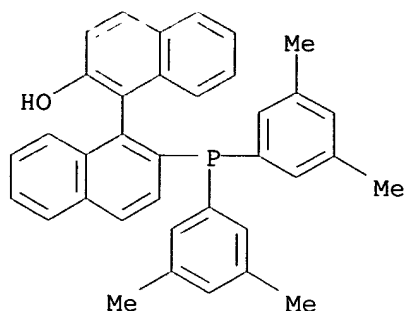
IT **149917-89-5P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for prepn. of binaphthalene phosphine-phosphinite compd. for asym. hydroformylation catalysis)

RN 149917-89-5 HCAPLUS

CN [1,1'-Binaphthalen]-2-ol, 2'-[bis(3,5-dimethylphenyl)phosphino]-, (R)- (9CI) (CA INDEX NAME)



L81 ANSWER 5 OF 18 HCAPLUS COPYRIGHT 2003 ACS
 AN 1996:610021 HCAPLUS
 DN 125:248105
 TI Optically active tertiary phosphine compounds, transition metal complexes comprising the same as ligands and process for preparing optically active organic silicon compounds using said transition metal complexes
 IN Hayashi, Tamio; Minai, Masayoshi; Iwakura, Kazunori
 PA Sumitomo Chemical Company Limited, Japan
 SO Eur. Pat. Appl., 20 pp.
 CODEN: EPXXDW

DT **Patent**

LA English

IC ICM C07F009-50

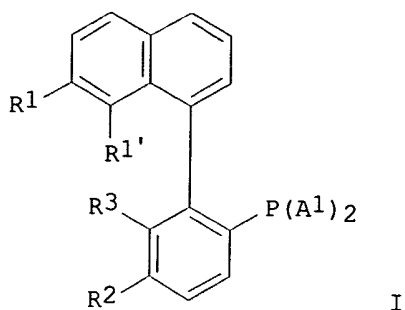
ICS B01J031-28; C07F015-00; C07F007-12

ICI C07M007-00

CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 25, 67

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 731105	A1	19960911	EP 1996-103689	19960308 <--
	EP 731105	B1	20011205		
	R: CH, DE, GB, LI				
	JP 08245662	A2	19960924	JP 1995-51094	19950310 <--
	JP 08245663	A2	19960924	JP 1995-51482	19950310 <--
	JP 09143185	A2	19970603	JP 1996-44680	19960301 <--
	US 5621129	A	19970415	US 1996-612108	19960307 <--
PRAI	JP 1995-49685	A	19950309	<--	
	JP 1995-51094	A	19950310	<--	
	JP 1995-51482	A	19950310	<--	
	JP 1995-238204	A	19950918	<--	
OS	CASREACT 125:248105; MARPAT 125:248105				
GI					



- AB The prepn. of tertiary phosphine compds. I ($R_1, R_1' = H, R_1R_1' = CH:CHCH:CH$; $R_2R_3 = 2-CH:CHC_6H_4$, etc.; $R_2 = H, R_3 =$ substituted or unsubstituted alkyl, Ph group, etc.; $A_1 = 3$ -trifluoromethylphenyl or 3,5-bis(trifluoromethyl)phenyl, etc.) was given. I was used as cocatalyst to prep. optically active silicon compd. Thus, (S)-3-diphenylphosphino-4,4'-biphenanthryl (prepn. given)/allylpalladium chloride dimer catalyzed silylation of styrene with trichlorosilane gave 1-phenyl-1-trichlorosilylethene. Oxidative desilylation of 1-phenyl-1-trichlorosilylethene with $KF/KHCO_3/H_2O_2$ in THF/MeOH gave optically pure (R)-1-phenethyl alc. in 95% yield.
- ST optically active phosphine compd prepn catalyst; transition metal catalyzed optically silicon prepn; asym synthesis aryl alc
- IT Asymmetric synthesis and induction
(prepn. of optically active tertiary phosphine compds. as cocatalysts for prepg. optically active org. silicon compds.)
- IT 85719-57-9
RL: CAT (Catalyst use); USES (Uses)
(Grignard phenylation of naphthylbis(trifluoromethanesulfonyloxy)benzene with phenylmagnesium bromide catalyzed by)
- IT 90-11-9, 1-Bromonaphthalene
RL: RCT (Reactant); RACT (Reactant or reagent)
(borylation of)
- IT 121-43-7, Trimethoxyborane
RL: RCT (Reactant); RACT (Reactant or reagent)
(borylation of bromonaphthalene with)
- IT 151-10-0, 1,3-Dimethoxybenzene
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)
- IT 7688-25-7, 1,4-Bis(diphenylphosphino)butane
RL: CAT (Catalyst use); USES (Uses)
(palladium-catalyzed phosphinylation of naphthylbis(trifluoromethanesulfonyloxy)benzene with diphenylphosphine oxide in presence of)
- IT 4559-70-0, Diphenylphosphine oxide
RL: RCT (Reactant); RACT (Reactant or reagent)
(phosphinylation of mesyloxybiphenanthryl compd. with)
- IT 1517-69-7P, (R)-1-Phenethyl alcohol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and carbamate formation of)
- IT 13922-41-3P, 1-Naphthylboric acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and coupling reaction with bromodimethoxybenzene)
- IT 16932-45-9P, 1-Bromo-2,6-dimethoxybenzene
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and coupling reaction with naphthylboric acid)
- IT 173300-93-1P, 1-Naphthyl-2,6-dimethoxybenzene

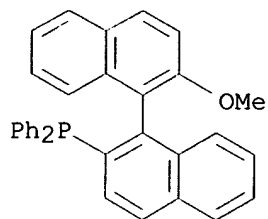
- RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and demethylation of)
- IT 170647-33-3P 181934-58-7P, (S)-3-Diphenylphosphinyl-4,4'-biphenanthryl
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deoxygenation of)
- IT 7726-28-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidative desilylation of)
- IT 181934-55-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and palladium catalyzed hydrogenation of)
- IT 170647-24-2P, 1-Naphthyl-2,6-bis(trifluoromethanesulfonyloxy)benzene
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and palladium-catalyzed phenylation of)
- IT 170647-29-7P 181934-57-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and phosphinylation of)
- IT 100838-76-4P, (R)-(-)-3,3'-Dihydroxy-4,4'-biphenanthryl 173300-94-2P, 1-Naphthyl-2,6-dihydroxybenzene 181934-56-5P, (S)-3-Hydroxy-4,4'-biphenanthryl
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and trifluoromethanesulfonylation of)
- IT 17995-58-3P 18035-34-2P 58276-68-9P 100838-77-5P, (S)-(+)-3,3'-Dihydroxy-4,4'-biphenanthryl 159241-56-2P 181934-63-4P, 3,5-Dinitrophenyl carbamate 181934-73-6P 181934-75-8P 181934-77-0P, 181934-99-6P 181935-04-6P 181935-08-0P 181935-10-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 12012-95-2, Allylpalladium chloride dimer **145964-33-6**
RL: CAT (Catalyst use); USES (Uses)
(prepn. of optically active tertiary phosphine compds. as cocatalysts for prepg. optically active org. silicon compds.)
- IT 156456-77-8P 170647-35-5P 181934-60-1P, (S)-3-Diphenylphosphino-4,4'-biphenanthryl 181934-89-4P 181934-90-7P 181934-92-9P 181934-94-1P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of optically active tertiary phosphine compds. as cocatalysts for prepg. optically active org. silicon compds.)
- IT 100-42-5, reactions 402-24-4, 3-Trifluoromethylphenylethene 402-50-6, 4-Trifluoromethylphenylethene 586-39-0, 3-Nitrophenylethene 611-15-4, 2-Methylphenylethene 622-97-9 637-50-3, 1-Phenylpropene 637-69-4 828-15-9, 1-Phenyl-1-hexene 1073-67-2, 4-Chlorophenylethene 2039-82-9, 4-Bromophenylethene 2039-85-2, 3-Chlorophenylethene 10025-78-2, Trichlorosilane 15929-44-9 15979-14-3 18531-94-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of optically active tertiary phosphine compds. as cocatalysts for prepg. optically active org. silicon compds.)
- IT 181934-84-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of optically active tertiary phosphine compds. as cocatalysts for prepg. optically active org. silicon compds.)
- IT 66478-70-4, 3,3'-Dihydroxy-4,4'-biphenanthryl
RL: RCT (Reactant); RACT (Reactant or reagent)
(racemic; optical resolu. of)
- IT **145964-33-6**

RL: CAT (Catalyst use); USES (Uses)

(prepn. of optically active tertiary phosphine compds. as cocatalysts
for prepg. optically active org. silicon compds.)

RN 145964-33-6 HCAPLUS

CN Phosphine, [(1R)-2'-methoxy[1,1'-binaphthalen]-2-yl]diphenyl- (9CI) (CA
INDEX NAME)



L81 ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2003 ACS

AN 1996:447108 HCAPLUS

DN 125:143006

TI Preparation of phosphine compounds as cocatalysts and their complexes as
catalysts for producing optically active aldehyde or the use of
4-[(R)-1'-formylethyl]azetidin-2-one derivatives as cocatalysts

IN Takaya, Hidemasa; Sakai, Nozomu; Tamao, Kyoko; Mano, Satoshi; Kumobayashi,
Hidenori; Tomita, Tetsuo; Saito, Takao; Matsumura, Kazuhiko; Kato,
Yasushi; Sayo, Noboru

PA Takasago International Corp., Japan

SO U.S., 29 pp., Cont.-in-part of U.S. Ser. No. 209,069, abandoned.

CODEN: USXXAM

DT **Patent**

LA English

IC ICM C07F015-00

ICS C07F009-02

NCL 556018000

CC 29-7 (Organometallic and Organometalloidal Compounds)

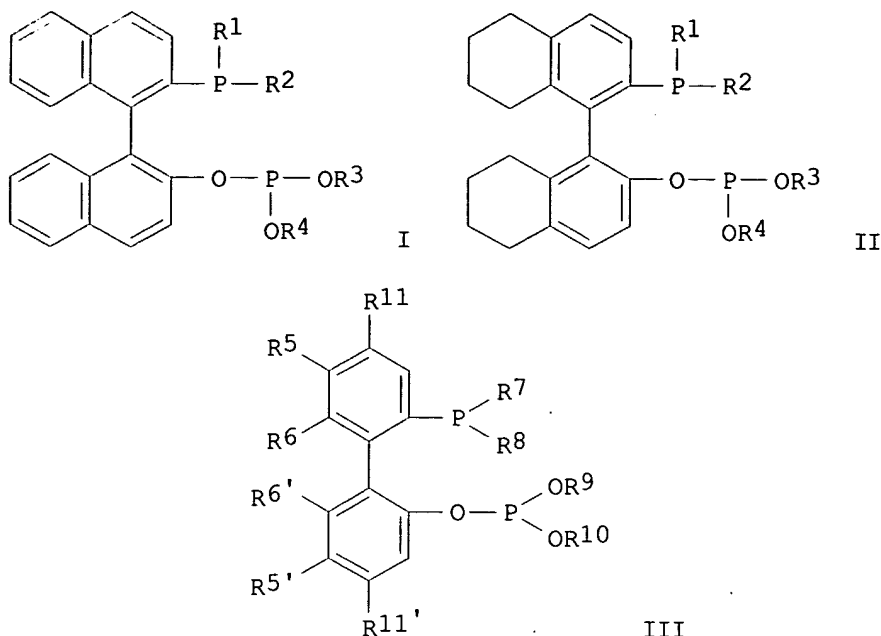
Section cross-reference(s): 21, 67

FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 5530150	A	19960625	US 1994-323492	19941012	<--
	JP 06263776	A2	19940920	JP 1993-52538	19930312	<--
	JP 3313805	B2	20020812			
	JP 06263681	A2	19940920	JP 1993-52539	19930312	<--
	JP 06263777	A2	19940920	JP 1993-52540	19930312	<--
	JP 2002128759	A2	20020509	JP 2001-328632	19940301	<--
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	JP 1993-52539	A	19930312			<--
	JP 1993-52540	A	19930312			<--
	JP 1993-77484	A	19930312			<--
	US 1994-208378	B2	19940310			<--
	US 1994-209051	B2	19940311			<--
	US 1994-209069	B2	19940311			<--
	US 1994-209070	B2	19940311			<--
	JP 1994-54426	A3	19940301			<--

OS CASREACT 125:143006; MARPAT 125:143006

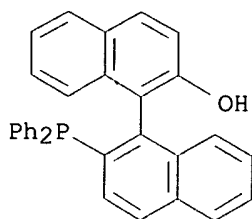
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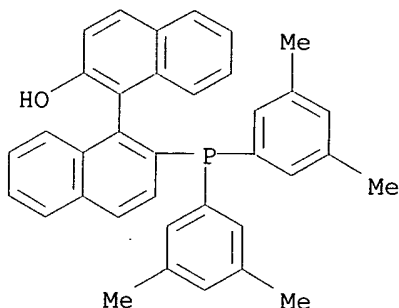
- AB The prepn. of phosphine compds. I-III (R^1, R^2 = same or different, each represent a Ph group or a Ph group substituted with a halogen atom or a lower alkyl group or taken together form a divalent hydrocarbon group; R^3, R^4 = same or different, each represent a lower alkyl group, a Ph group or a Ph group substituted with a halogen atom, a lower alkyl group or a lower alkoxy group or taken together form a divalent hydrocarbon group; $\text{R}^6, \text{R}^{6'}$ = same or different, each represent H, lower alkyl group or lower alkoxy group; $\text{R}^5, \text{R}^{5'}, \text{R}^{11}, \text{R}^{11'}$ = same or different, each represent H, lower alkyl group, lower alkoxy group, halogen atom; or a pair of R^5 and R^6 or a pair of $\text{R}^{5'}$ and $\text{R}^{6'}$ may form a ring; R^7, R^8 = same or different, each represent a Ph group or a Ph group substituted with a lower alkyl group, a halogen atom or a lower alkoxy group; $\text{R}^9, \text{R}^{10}$ = same or different, each represent a Ph group or a Ph group substituted with a lower alkyl group, a lower alkoxy group or a halogen atom; or R^9 and R^{10} may be taken together to form a divalent hydrocarbon group) and their transition metal complexes, useful in the prepn. of optically active aldehydes, is described. Thus, title phosphine (R)-2-diphenylphosphino-1,1'-binaphthalene-2'-yloxy-((S)-1,1'-binaphthalene-2,2'-diyldioxy)phosphine [(R,S)-BINAPHOS] prep'd. in 5 steps starting from (R)-1,1'-bi-2-naphthol. [(R,S)-BINAPHOS]/Rh(CO)₂(acac) catalyzed asym. hydroformylation of vinyl acetate gave 2-acetoxypionic acid predominantly which upon Jones oxidn. gave (S)-(-)-2-acetoxypionic acid with 99% enantiomeric excess.
- ST phosphine ligand prepn cocatalyst asym hydroformylation; BINAPHOS prepn cocatalyst asym hydroformylation; rhodium catalyst phosphine ligand cocatalyst hydroformylation; aldehyde optically active prepn
- IT Aldehydes, preparation
- RL: SPN (Synthetic preparation); PREP (Preparation)
(optically active; prepn. of phosphine compds. as cocatalysts and its complexes as catalysts for producing optically active aldehyde)
- IT Asymmetric synthesis and induction
(prepn. of phosphine compds. as cocatalysts and its complexes as catalysts for producing optically active aldehyde)
- IT Hydroformylation catalysts
(asym., prepn. of phosphine compds. as cocatalysts and its complexes as catalysts for producing optically active aldehyde)
- IT Hydroformylation

- (stereoselective, prepn. of phosphine compds. as cocatalysts and its complexes as catalysts for producing optically active aldehyde)
- IT 104-53-0P, Benzenepropanal 111-71-7P, Heptanal 2436-29-5P 5406-12-2P
6034-46-4P, (S)-(-)-2-Acetoxypropionic acid 7782-24-3P,
(S)-(+)-2-Phenylpropionic acid 18545-28-3P 20401-88-1P 33204-48-7P
37414-44-1P 38235-74-4P 40764-03-2P 66875-69-2P 66875-71-6P
73365-03-4P 75677-02-0P 81292-68-4P 110773-62-1P 132151-88-3P
147922-82-5P 149917-84-0P 155566-54-4P 159496-97-6P 180060-81-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 159496-98-7P 159573-35-0P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of formylethylazetidinone derivs. as cocatalysts for producing optically active aldehyde)
- IT 112256-72-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of formylethylazetidinone derivs. as cocatalysts for producing optically active aldehyde)
- IT 12092-47-6 159398-11-5 179893-92-6 180060-82-6 180060-83-7
RL: CAT (Catalyst use); USES (Uses)
(prepn. of phosphine compds. as cocatalysts and its complexes as catalysts for producing optically active aldehyde)
- IT 14874-82-9, (Acetylacetonato)dicarbonylrhodium
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(prepn. of phosphine compds. as cocatalysts and its complexes as catalysts for producing optically active aldehyde)
- IT 149917-85-1P 149917-86-2P 149917-87-3P 149952-92-1P 149952-93-2P
155566-52-2P 155566-53-3P 155613-50-6P 155613-51-7P 159496-88-5P
159496-91-0P 159496-94-3P 159573-28-1P 159573-29-2P 159573-30-5P
159573-31-6P 159573-32-7P 159573-33-8P 159573-34-9P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of phosphine compds. as cocatalysts and its complexes as catalysts for producing optically active aldehyde)
- IT 159398-04-6P 159398-05-7P 159398-06-8P 159398-07-9P 159398-08-0P
159398-09-1P 159398-10-4P 159398-23-9P 159398-24-0P 159398-26-2P
159436-33-6P 159496-96-5P 159516-49-1P 159516-54-8P 159516-55-9P
159516-56-0P 159518-56-6P 179893-91-5P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of phosphine compds. as cocatalysts and its complexes as catalysts for producing optically active aldehyde)
- IT 88-04-0, 4-Chloro-3,5-xylene 95-13-6, 1H-Indene 100-42-5, reactions
107-01-7, 2-Butene 108-05-4, Acetic acid ethenyl ester, reactions
447-53-0 527-54-8, 3,4,5-Trimethylphenol 592-41-6, 1-Hexene, reactions
622-97-9 637-69-4 1073-67-2 3485-84-5 4559-70-0, Diphenylphosphine oxide 5382-00-3, Chlorodiphenoxyphosphine 18531-94-7 18531-99-2,
(S)-1,1'-Bi-2-naphthol 63444-56-4 65355-00-2 95033-74-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of phosphine compds. as cocatalysts and its complexes as catalysts for producing optically active aldehyde)
- IT 17763-95-0P 33530-47-1P 34638-21-6P 65355-14-8P 66875-70-5P
126613-06-7P 132532-04-8P 137156-22-0P 149917-88-4P
149917-89-5P 155566-46-4P 155566-47-5P 155566-48-6P
155566-49-7P 155566-50-0P 155566-51-1P 155613-52-8P 159496-89-6P
159496-90-9P 159496-92-1P 159496-93-2P 159496-95-4P 179893-88-0P
179893-89-1P 179893-90-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of phosphine compds. as cocatalysts and its complexes as catalysts for producing optically active aldehyde)

IT 149917-88-4P 149917-89-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. of phosphine compds. as cocatalysts and its complexes as
 catalysts for producing optically active aldehyde)
 RN 149917-88-4 HCAPLUS
 CN [1,1'-Binaphthalen]-2-ol, 2'-(diphenylphosphino)-, (1R)- (9CI) (CA INDEX
 NAME)



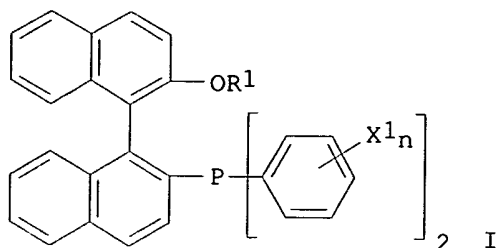
RN 149917-89-5 HCAPLUS
 CN [1,1'-Binaphthalen]-2-ol, 2'-[bis(3,5-dimethylphenyl)phosphino]-, (R)-
 (9CI) (CA INDEX NAME)



L81 ANSWER 7 OF 18 HCAPLUS COPYRIGHT 2003 ACS
 AN 1996:169300 HCAPLUS
 DN 124:343650
 TI Optically active tertiary phosphines, their metal complexes, and
 preparation of optically active organosilicon compounds
 IN Iwakura, Kazunori; Minamii, Masayoshi
 PA Sumitomo Chemical Co, Japan
 SO Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DT **Patent**
 LA Japanese
 IC ICM C07F009-50
 ICS B01J031-18; C07F007-14; C07F007-18
 ICA C07B061-00
 ICI C07M007-00
 CC 29-6 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 67

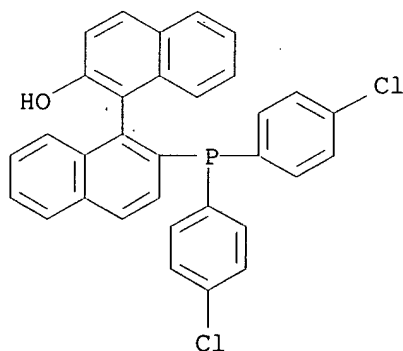
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 07330786	A2	19951219	JP 1994-127786	19940609 <--
PRAI	JP 1994-127786		19940609 <--		
OS	CASREACT 124:343650; MARPAT 124:343650				
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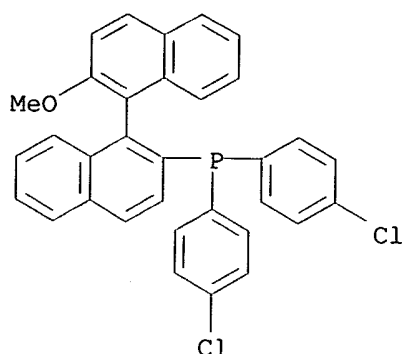


- AB The tertiary phosphines I ($R_1 = H$, lower alkyl which may be substituted with halo, lower alkoxy, Ph; $X_1 = \text{halo}$; $n = 1-5$) and transition metal complexes having I as the ligands are claimed. Also claimed is a method for the prepn. of optically active $R_2R_3CHCR_4R_5SiX_2X_3X_4$ ($R_2-5 = \text{alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, alkoxy, H}$; 2 of them may be linked each other to form a ring; $X_2-4 = H, \text{alkyl, alkoxy, halo}$), useful as synthetic intermediates, by treatment of $R_2R_3C:CR_4R_5$ with $X_2X_3X_4SiH$ in the presence of transition metal complexes having I as the ligands. (4-ClC₆H₄)₂P(O)H (prepn. given) was treated with (R)-2,2'-bis(trifluoromethanesulfonyloxy)-1,1'-binaphthyl (prepn. given) to give (R)-2-trifluoromethanesulfonyloxy-2'-bis(4-chlorophenyl)phosphinoyl-1,1'-binaphthyl, which was hydrolyzed followed by O-methylation and redn. to give (R)-I ($R_1 = Me, X_1 = 4-Cl$) (II). A toluene soln. of allylpalladium chloride dimer and II was treated with norbornene and SiHCl₃ under stirring for 12 h to give 97% (1S,2S,4R)-2-trichlorosilylnorbornane with 95% e.e., vs. 95 and 89% e.e. for a control prep. using (R)-(+)-2-diphenylphosphino-2'-methoxy-1,1'-binaphthyl as a ligand.
- ST halophenylphosphinobinaphthyl prepn ligand hydrosilylation catalyst; phsophinobinaphthyl halophenylphosphino ligand hydrosilylation catalyst; optically active organosilicon compd prepn
- IT Hydrosilylation catalysts
([bis(halophenyl)phosphino]binaphthyl transition metal complexes)
- IT Alkenes, reactions
Cycloalkenes
Silanes
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. hydrosilylation of (cyclo)alkenes with silanes using [bis(halophenyl)phosphino]binaphthyl transition metal complexes)
- IT 176370-78-8P, (R)-2-Hydroxy-2'-[bis(4-chlorophenyl)phosphino]-1,1'-binaphthyl
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
([bis(halophenyl)phosphino]binaphthyl transition metal complexes as asym. hydrosilylation catalysts)
- IT 358-23-6, Trifluoromethanesulfonic anhydride 637-87-6,
1-Chloro-4-iodobenzene 762-04-9, Diethyl phosphite 122531-87-7,
(R)-.beta.-Binaphthol
RL: RCT (Reactant); RACT (Reactant or reagent)
([bis(halophenyl)phosphino]binaphthyl transition metal complexes as asym. hydrosilylation catalysts)
- IT 15948-60-4P, Bis(4-chlorophenyl)phosphine oxide 126613-06-7P,
(R)-2,2'-Bis(trifluoromethanesulfonyloxy)-1,1'-binaphthyl 176370-75-5P,
(R)-2-(Trifluoromethanesulfonyloxy)-2'-[bis(4-chlorophenyl)phosphinoyl]-1,1'-binaphthyl 176370-76-6P, (R)-2-Hydroxy-2'-[bis(4-chlorophenyl)phosphinoyl]-1,1'-binaphthyl 176370-77-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
([bis(halophenyl)phosphino]binaphthyl transition metal complexes as asym. hydrosilylation catalysts)

- IT 146075-48-1P, (1S,2S,4R)-2-(Trichlorosilyl)norbornane
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (asym. hydrosilylation of (cyclo)alkenes with silanes using [bis(halophenyl)phosphino]binaphthyl transition metal complexes)
- IT 498-66-8, Bicyclo[2.2.1]hept-2-ene 10025-78-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (asym. hydrosilylation of (cyclo)alkenes with silanes using [bis(halophenyl)phosphino]binaphthyl transition metal complexes)
- IT 12012-95-2, Allylpalladium chloride dimer
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts contg. (R)-2-methoxy-2'-[bis(4-chlorophenyl)phosphino]-1,1'-binaphthyl; asym. hydrosilylation catalyst)
- IT 165730-08-5P, (R)-2-Methoxy-2'-[bis(4-chlorophenyl)phosphino]-1,1'-binaphthyl
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (catalysts contg. allylpalladium chloride dimer; [bis(halophenyl)phosphino]binaphthyl transition metal complexes as asym. hydrosilylation catalysts)
- IT 61277-93-8P, (1S,2S,4R)-2-Norbornanol
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of norbornanol from (trichlorosilyl)norbornane)
- IT 176370-78-8P, (R)-2-Hydroxy-2'-[bis(4-chlorophenyl)phosphino]-1,1'-binaphthyl
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 ([bis(halophenyl)phosphino]binaphthyl transition metal complexes as asym. hydrosilylation catalysts)
- RN 176370-78-8 HCAPLUS
 CN [1,1'-Binaphthalen]-2-ol, 2'-[bis(4-chlorophenyl)phosphino]-, (R)- (9CI)
 (CA INDEX NAME)



- IT 165730-08-5P, (R)-2-Methoxy-2'-[bis(4-chlorophenyl)phosphino]-1,1'-binaphthyl
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (catalysts contg. allylpalladium chloride dimer; [bis(halophenyl)phosphino]binaphthyl transition metal complexes as asym. hydrosilylation catalysts)
- RN 165730-08-5 HCAPLUS
 CN Phosphine, bis(4-chlorophenyl) (2'-methoxy[1,1'-binaphthalen]-2-yl)-, (R)- (9CI) (CA INDEX NAME)



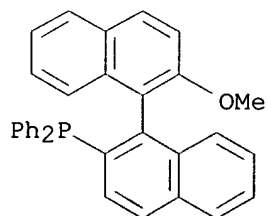
L81 ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2003 ACS
 AN 1996:137584 HCAPLUS
 DN 124:176140
 TI Preparation of optically active heteroarylalkanol and arylalkanol
 IN Azumai, Takayuki; Minamii, Masayoshi; Fujimoto, Yukari; Matsumoto, Tsutomu
 PA Sumitomo Chemical Co, Japan
 SO Jpn. Kokai Tokkyo Koho, 14 pp.
 CODEN: JKXXAF
 DT **Patent**
 LA Japanese
 IC ICM C07D239-26
 ICS B01J031-24; C07C029-48; C07C033-24; C07C033-46; C07C041-30;
 C07C043-23; C07D213-06; C07D213-30; C07D215-20; C07D217-02;
 C07D237-08; C07D239-34; C07D239-74; C07D239-80; C07D241-12;
 C07D241-44; C07D401-04; C07D401-10; C07D403-04
 CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 07291940	A2	19951107	JP 1994-89663	19940427 <--
PRAI	JP 1994-89663		19940427 <--		
OS	CASREACT 124:176140; MARPAT 124:176140				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compd. represented by formula $R_1(O)mA_1(A_2)pA_3(CH_2)nR$ [I; R = CH(OH)Me; R_1 = C1-20 (halo)alkyl, C2-20 (halo)alkoxyalkyl; A_1 , A_2 , A_3 = Q - Q9; wherein u, w = 0-3; provided that when A_1 = fused ring, A_2 = monocyclic ring or when A_1 = monocyclic ring and p = 1, A_2 and A_3 = monocyclic ring; n = 0-10; m, p = 0,1], useful as an intermediate for agrochems., drugs and ferroelec. liq. crystals, is prepd. by hydrosilylation of an α -alkene I (R = CH:CH₂) with HSi(X₅)₃ (X₅ = H, alkyl, alkoxy, halo) in the presence of a transition metal complex having an optically active tert-phosphine binaphthyl compd. [R₂ = halo, alkoxy, alkoxyalkoxy, (phenyl)alkyl, C5-7 cycloalkyl; R₃ = alkyl, alkoxy, (halo)phenyl; R₄, R₅ = H, alkyl; or R₄R₅ forms a fused ring] and oxidn. of the resulting silane I [R = CHMeSi(X₅)₃]. Thus, 5.4 g trichlorosilane was slowly added dropwise to a mixt. of 10 g 2-[4-(5-hexen-1-yl)phenyl]-5-octyloxypyrimidine, 0.46 mg π -allylpalladium chloride, and 1.22 mg (S)-I (R₂ = Me, R₃ = Ph, R₄ = R₅ = H) at 25-30.degree. and the resulting mixt. was stirred for 10 h and added to a suspension of 1.7 g KF and 9 g KHCO₃ in 100 mL THF and 100 mL MeOH under ice-cooling. The resulting

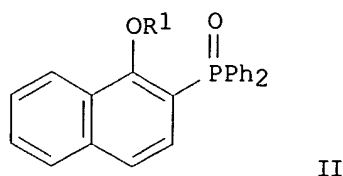
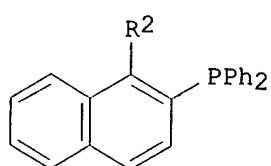
- mixt. was stirred under ice-cooling for 2 h, followed by adding 25 mL 30% H₂O₂, and the reaction mixt. was stirred at 50.degree. for 24 h to give, after silica gel chromatog., the optically active title compd. [(-)-II].
- ST heteroarylalkanol optically active prepn; arylalkanol optically active prepn; allylpalladium chloride stereoselective hydrosilylation catalyst; phosphinobinaphthyl hydrosilylation catalyst ligand; trichlorosilane hydrosilylation alkene
- IT Hydrosilylation catalysts
(stereoselective, allylpalladium chloride and phosphinobinaphthyl deriv.; prepn. of optically active heteroarylalkanol and arylalkanol by hydrosilylation of heteroaryl- or aryl-.alpha.-alkene with trichlorosilane)
- IT Hydrosilylation
(stereoselective, prepn. of optically active heteroarylalkanol and arylalkanol by hydrosilylation of heteroaryl- or aryl-.alpha.-alkene with trichlorosilane)
- IT 12012-95-2, .pi.-Allylpalladium chloride **134484-36-9**
RL: CAT (Catalyst use); USES (Uses)
(prepn. of optically active heteroarylalkanol and arylalkanol by hydrosilylation of heteroaryl- or aryl-.alpha.-alkene with trichlorosilane)
- IT 10025-78-2 165320-52-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of optically active heteroarylalkanol and arylalkanol by hydrosilylation of heteroaryl- or aryl-.alpha.-alkene with trichlorosilane)
- IT 174073-63-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of optically active heteroarylalkanol and arylalkanol by hydrosilylation of heteroaryl- or aryl-.alpha.-alkene with trichlorosilane)
- IT **134484-36-9**
RL: CAT (Catalyst use); USES (Uses)
(prepn. of optically active heteroarylalkanol and arylalkanol by hydrosilylation of heteroaryl- or aryl-.alpha.-alkene with trichlorosilane)
- RN 134484-36-9 HCAPLUS
- CN Phosphine, [(1S)-2'-methoxy[1,1'-binaphthalen]-2-yl]diphenyl- (9CI) (CA INDEX NAME)



- L81 ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2003 ACS
- AN 1995:777644 HCAPLUS
- DN 123:199144
- TI Preparation of 1-substituted-2-(diphenylphosphino)naphthalenes
- IN Myano, Sotaro; Hatsutori, Tetsutaro; Sakamoto, Junichi
- PA Sumitomo Seika Kk, Japan
- SO Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
- DT Patent
- LA Japanese
- IC ICM C07F009-50

CC 29-7 (Organometallic and Organometalloidal Compounds)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06256367	A2	19940913	JP 1993-49703	19930310 <--
PRAI	JP 1993-49703		19930310		
OS	CASREACT 123:199144; MARPAT 123:199144				
GI					



AB Title compds. I (R2 = alkyl, aralkyl, aryl, alkoxy, alkylamino) were prep'd. from 1-alkoxy-2-(oxodiphenylphosphino)naphthalenes II (R1 = alkyl, aralkyl) by reaction with nucleophiles followed by redn. Thus, reaction of 1-methoxy-2-(oxodiphenylphosphino)naphthalene with NaOMe in DMF gave 78% 1-butoxy-2-(oxodiphenylphosphino)naphthalene, redn of which with HSiCl3 and Et3N in xylene gave 99% 1-butoxy-2-(diphenylphosphino)naphthalene.

ST phosphine triaryl; phenylphosphinonaphthalene; naphthalene diphenylphosphino

IT 90-15-3, 1-Naphthol 109-72-8, reactions 683-60-3, Sodium isopropoxide 693-03-8, n-Butylmagnesium bromide 1079-66-9, Chlorodiphenylphosphine 2372-45-4, Sodium butoxide 4111-54-0, Lithium diisopropylamide 16750-63-3, 2-Methoxyphenylmagnesium bromide 20752-47-0 27303-99-7, (-)-Menthyl sodium salt 36321-90-1, 2-Methoxy-1-naphthylmagnesium bromide 167363-32-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of (diphenylphosphino)naphthalenes)

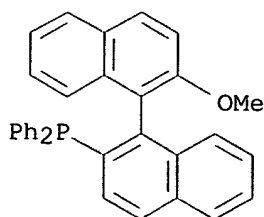
IT 2216-69-5P, 1-Methoxynaphthalene 161053-37-8P 161053-38-9P
161053-42-5P 161053-43-6P 161053-45-8P 161053-51-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of (diphenylphosphino)naphthalenes)

IT 161053-32-3P 161053-34-5P 161053-39-0P 161053-44-7P
161053-46-9P 161053-47-0P 161053-48-1P 161053-49-2P
167363-33-9P 167363-34-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of (diphenylphosphino)naphthalenes)

IT **161053-46-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of (diphenylphosphino)naphthalenes)

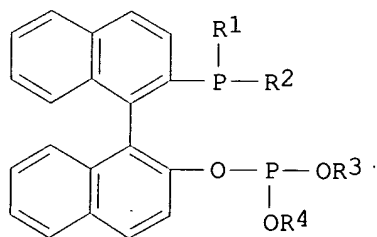
RN 161053-46-9 HCAPLUS

CN Phosphine, (2'-methoxy[1,1'-binaphthalen]-2-yl)diphenyl- (9CI) (CA INDEX NAME)



L81 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2003 ACS
 AN 1995:742567 HCAPLUS
 DN 123:198277
 TI Process and chiral rhodium hydroformylation catalysts for preparing optically active aldehydes.
 IN Takaya, Hidemasa; Sakai, Nozomu; Tamao, Kyoko Beru; Mano, Satoshi; Kumobayashi, Hidenori; Tomita, Tetsuo
 PA Mitsubishi Gas Chemical Co., Inc., Japan; Takasago International Corp.
 SO Eur. Pat. Appl., 12 pp.
 CODEN: EPXXDW
 DT **Patent**
 LA English
 IC ICM C07C045-50
 ICS C07C045-49; C07C047-14; C07C047-228; C07C047-277; C07C067-293; C07C069-14; C07D209-48; C07C253-30; C07C255-17
 CC 23-14 (Aliphatic Compounds)
 Section cross-reference(s): 67
 FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 614870	A2	19940914	EP 1994-103675	19940310 <--
	EP 614870	A3	19941109		
	EP 614870	B1	19980114		
	R: DE, FR, GB				
	JP 06263681	A2	19940920	JP 1993-52539	19930312 <--
PRAI	JP 1993-52539	A	19930312	<--	
OS	CASREACT 123:198277; MARPAT 123:198277				
GI					



AB Optically active aldehydes $\text{OHCCH}(\text{CH}_3)\text{Q}$ [Q = halogen, lower alkyl, phthalimido, lower alkylcarbonyloxy, CN, (un)substituted Ph, etc.] [e.g., (S)-2-phenylpropanal], which are expensively synthesized using prior-art techniques, can be produced in high yield and at low cost by hydroformylating an olefin $\text{H}_2\text{C:CHQ}$ (e.g., vinyl acetate) in the presence of a rhodium catalyst system contg. a chiral phosphine ligand [I; R1, R2 = (un)substituted Ph; R3, R4 = lower alkyl, (un)substituted Ph].

ST catalyst rhodium asym hydroformylation; chiral aldehyde prepn asym hydroformylation alkene

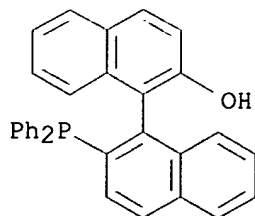
IT Hydroformylation catalysts
 (asym., chiral rhodium complexes for prepg. optically active aldehydes)

IT Aldehydes, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (chiral, process and chiral rhodium hydroformylation catalysts for prepg.)

IT Hydroformylation
 (stereoselective, prepg. optically active aldehydes by)

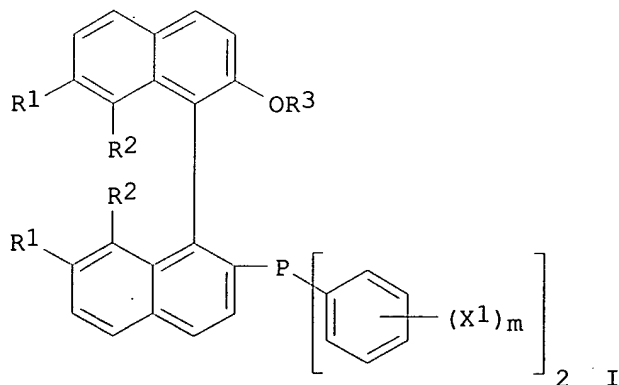
IT 4559-70-0, Diphenylphosphine oxide 6737-42-4, 1,3-Bis(diphenylphosphino)propane 14874-82-9 18531-94-7,

- (R)-1,1'-Bi-2-naphthol 18531-99-2, (S)-1,1'-Bi-2-naphthol 155613-52-8
 RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
 (catalyst precursor; process and chiral rhodium hydroformylation catalysts for prepg. optically active aldehydes)
- IT 126613-06-7P 132532-04-8P 137156-22-0P 149917-85-1P
149917-88-4P 149952-92-1P
 RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (catalyst precursor; process and chiral rhodium hydroformylation catalysts for prepg. optically active aldehydes)
- IT 104-53-0P, 3-Phenylpropanal 18545-28-3P, 3-Acetoxypopropanal
 RL: BYP (Byproduct); PREP (Preparation)
 (process and chiral rhodium hydroformylation catalysts for prepg. optically active aldehydes)
- IT 159516-56-0
 RL: CAT (Catalyst use); USES (Uses)
 (process and chiral rhodium hydroformylation catalysts for prepg. optically active aldehydes)
- IT 75-01-4, Vinyl chloride, reactions 100-42-5, Styrene, reactions
 107-13-1, Acrylonitrile, reactions 108-05-4, Vinyl acetate, reactions
 622-97-9, 4-Methylstyrene 630-08-0, Carbon monoxide, reactions
 637-69-4, 4-Methoxystyrene 1073-67-2, 4-Chlorostyrene 26206-42-8,
 4-Butylstyrene 63444-51-9, 2-Methoxy-6-vinylnaphthalene 63444-56-4,
 4-Isobutylstyrene 84494-80-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (process and chiral rhodium hydroformylation catalysts for prepg. optically active aldehydes)
- IT 33530-47-1P, (S)-2-Phenylpropanal 66875-70-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (process and chiral rhodium hydroformylation catalysts for prepg. optically active aldehydes)
- IT 111-71-7P, Heptanal 5406-12-2P 6034-46-4P 7782-24-3P,
 (S)-(+)-2-Phenylpropionic acid 20401-88-1P 40764-03-2P 75677-02-0P
 110773-62-1P 122091-55-8P 132151-88-3P 147922-82-5P 149917-84-0P
 166587-68-4P 166587-69-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (process and chiral rhodium hydroformylation catalysts for prepg. optically active aldehydes)
- IT **149917-88-4P**
 RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (catalyst precursor; process and chiral rhodium hydroformylation catalysts for prepg. optically active aldehydes)
- RN 149917-88-4 HCAPLUS
 CN [1,1'-Binaphthalen]-2-ol, 2'-(diphenylphosphino)-, (1R)- (9CI) (CA INDEX NAME)



DN 123:144274
 TI Preparation of tertiary phosphines and their transition metal complexes as catalysts for asymmetric synthesis reactions
 IN Hayashi, Tamio; Uozumi, Yasuhiro; Iwakura, Kazunori; Kurimoto, Isao; Minai, Masayoshi
 PA Sumitomo Chemical Co., Ltd., Japan
 SO Eur. Pat. Appl., 21 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 IC ICM C07F009-50
 ICS B01J031-28; C07F015-00; C07F007-08; C07F007-14; C07F007-18; C07C001-22
 ICI C07M005-00, C07M007-00
 CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 21
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 647647	A1	19950412	EP 1994-111780	19940728 <--
	EP 647647	B1	20011024		
	R: CH, DE, FR, GB, LI				
	JP 07149776	A2	19950613	JP 1994-15341	19940209 <--
	JP 07224073	A2	19950822	JP 1994-16760	19940210 <--
	US 5523437	A	19960604	US 1994-280814	19940726 <--
PRAI	JP 1993-251635	A	19931007	<--	
	JP 1994-15341	A	19940209	<--	
	JP 1994-16760	A	19940210	<--	
OS	MARPAT 123:144274				
GI					



AB The prepn. of tertiary phosphine compd. I (R1, R2 = independently from each other a H, Me; R1R2 = CH:CHCH:CH; R3 = H, C5-7 cycloalkyl, lower alkyl group which may be substituted with halogen, lower alkoxy, lower alkoxyalkoxy, Ph; X1 = halogen atom when both R1 and R2 are hydrogens, hydrogen atom, halogen atom, lower alkyl group, lower alkoxy group when at least one of R1 and R2 is not a hydrogen atoms; m = 1-5), useful as ligand of a transition metal complex that can catalyze various reactions, is described. Thus, redn. of (R)-(+)-3-diphenylphosphinyl-3'-methoxy-4,4'-biphenanthryl (prepn. given) with HSiCl3 in the presence of Et3N gave title compd., (R)-(+)-3-diphenylphosphino-3'-methoxy-4,4'-biphenanthryl (II), which was used in asym. synthesis of .alpha.-olefins. Thus, tris(dibenzylideneacetone) (chloroform)dipalladium(0)-catalyzed reaction of

- geranylmethyl carbonate with formic acid in the presence of 1,8-bis(dimethylamino)naphthalene and chiral cocatalyst II gave (S)-3,7-dimethyl-1,6-octadiene.
- ST tertiary phosphine prepn cocatalyst asym synthesis; biphenanthryl phosphine prepn cocatalyst asym synthesis; palladium phosphine complex catalyst asym synthesis
- IT Catalysts and Catalysis
(asym. synthesis; prepn. of tertiary phosphines and their transition metal complexes as catalysts for asym. synthesis reactions)
- IT Asymmetric synthesis and induction
(prepn. of tertiary phosphines and their transition metal complexes as catalysts for asym. synthesis reactions)
- IT 26593-50-0, 2-Hydroxy-7-methylnaphthalene
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidn. of)
- IT 4559-70-0, Diphenylphosphine oxide
RL: RCT (Reactant); RACT (Reactant or reagent)
(phosphonylation of trifloxybiphenanthryl with)
- IT 1115-82-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and anilide formation of)
- IT 103981-06-2P, (S)-3-Triethylsilyl-1-butene
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and carbamylation of)
- IT 157397-73-4P 165730-04-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)
- IT 157397-74-5P 165730-05-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and methylation of)
- IT 10281-55-7P, (S)-3,7-Dimethyl-1,6-octadiene 146075-48-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)
- IT 18531-94-7P 157397-72-3P 165730-03-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and phosphonylation of)
- IT 157397-75-6P 165730-06-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
- IT 157584-78-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and resolu. of)
- IT 100838-76-4P, (R)-(-)-3,3'-Dihydroxy-4,4'-biphenanthryl 157584-79-7P, (R)-(+)-2,2'-Dihydroxy-7,7'-dimethyl-1,1'-binaphthyl
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and triflation of)
- IT 10281-56-8P, (R)-3,7-Dimethyl-1,6-octadiene 36617-88-6P 61277-93-8P 84170-98-9P 100838-77-5P, (S)-(+)-3,3'-Dihydroxy-4,4'-biphenanthryl 125847-56-5P, (R)-3-Cyclohexyl-1-butene 153279-32-4P 157397-77-8P 157397-78-9P 157584-80-0P, (S)-(-)-2,2'-Dihydroxy-7,7'-dimethyl-1,1'-binaphthyl 161550-38-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 6737-42-4 12012-95-2 51364-51-3

RL: CAT (Catalyst use); USES (Uses)

(prepn. of tertiary phosphines and their transition metal complexes as catalysts for asym. synthesis reactions)

IT 155184-93-3P 165730-07-4P 165730-08-5P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. of tertiary phosphines and their transition metal complexes as catalysts for asym. synthesis reactions)

IT 20734-58-1, 1,8-Bis(dimethylamino)naphthalene

RL: NUU (Other use, unclassified); USES (Uses)

(prepn. of tertiary phosphines and their transition metal complexes as catalysts for asym. synthesis reactions)

IT 498-66-8, Bicyclo[2.2.1]hept-2-ene 630-19-3, Pivalic aldehyde

85217-72-7, Geranylmethyl carbonate 85217-73-8 155184-90-0

157397-76-7 158261-40-6 158261-41-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of tertiary phosphines and their transition metal complexes as catalysts for asym. synthesis reactions)

IT 158261-46-2P, (R)-3-Phenyl-3-triethylsilyl-1-propene

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of tertiary phosphines and their transition metal complexes as catalysts for asym. synthesis reactions)

IT 100780-04-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(resoln. of)

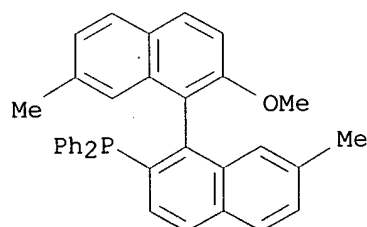
IT 165730-07-4P 165730-08-5P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. of tertiary phosphines and their transition metal complexes as catalysts for asym. synthesis reactions)

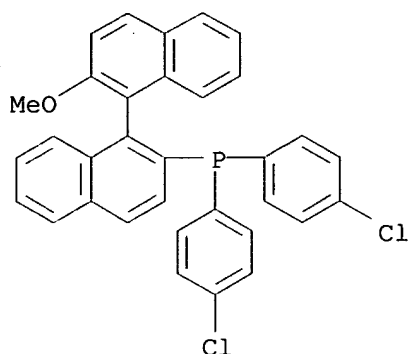
RN 165730-07-4 HCAPLUS

CN Phosphine, (2'-methoxy-7,7'-dimethyl[1,1'-binaphthalen]-2-yl)diphenyl-,
(R)- (9CI) (CA INDEX NAME)



RN 165730-08-5 HCAPLUS

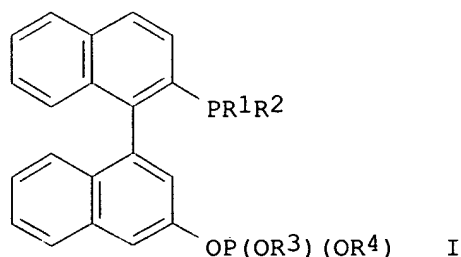
CN Phosphine, bis(4-chlorophenyl)(2'-methoxy[1,1'-binaphthalen]-2-yl)-, (R)-
(9CI) (CA INDEX NAME)



L81 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2003 ACS
 AN 1995:231203 HCAPLUS
 DN 122:10257
 TI preparation of phosphine compounds and their transition metal complexes
 IN Takaya, Hidemasa; Sakai, Nozomu; Tamao, Kyoko Beru Mezon; Mano, Satoshi;
 Kumobayashi, Hidenor; Tomita, Tetsu
 PA Mitsubishi Gas Chemical Company, Inc., Japan; Takasago International
 Corporation
 SO Eur. Pat. Appl., 12 pp.
 CODEN: EPXXDW
 DT **Patent**
 LA English
 IC ICM C07F009-50
 ICS C07F015-00; C07C045-50; C07F009-6574; C07F009-6568
 CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 67, 78

FAN.CNT 5

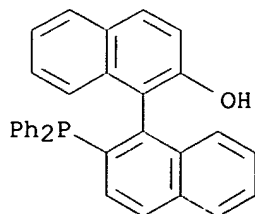
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 614901	A1	19940914	EP 1994-103674	19940310 <--
	EP 614901	B1	19980812		
	R: CH, DE, FR, GB, IT, LI, NL				
	JP 06263776	A2	19940920	JP 1993-52538	19930312 <--
	JP 3313805	B2	20020812		
PRAI	JP 1993-52538	A	19930312	<--	
OS	CASREACT 122:10257; MARPAT 122:10257				
GI					



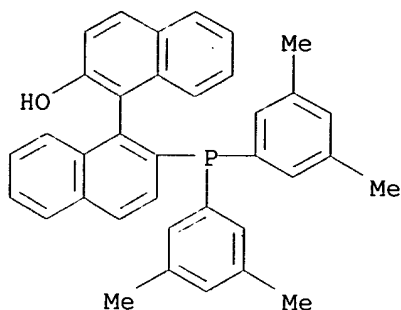
AB Disclosed herein is the prepn. of phosphine compd. I (R1, R2 = same or different halo or lower alkyl group substituted Ph, divalent hydrocarbon group; R3, R4 = same or different alkyl, halo or lower alkyl group substituted Ph, divalent hydrocarbon group), and their transition metal-phosphine complexes. When the transition metal-phosphine complex is

used as a catalyst for asym. synthesis, an intended product having a desired abs. configuration can be obtained in a high optical purity at a high yield. Thus, reaction of (R)-2-diphenylphosphino-2'-hydroxy-1,1'-binaphthyl (prepn. given) with (S)-1,1'-binaphthalene-2,2'-diyldioxychlorophosphine (prepn. given) in the presence of Et₃N in Et₂O gave 98% title phosphine, (R)-2-diphenylphosphino-1,1'-binaphthalene-2'-yloxy((S)-1,1'-binaphthalene-2,2'-diyldioxy)phosphine, which was reacted with [Rh(CO)₂(acac)] to give asym. hydroformylation catalyst for vinyl acetate or styrene.

- ST diposphine prep transition metal ligand; rhodium diposphine complex
prepn hydroformylation catalyst
- IT Hydroformylation catalysts
(asym., prep. of phosphine compds. and their transition metal complexes)
- IT 104-53-0P, Benzenepropanal 18545-28-3P 33530-47-1P 66875-70-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)
- IT 6034-46-4P 7782-24-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 100-42-5, reactions 108-05-4, Acetic acid ethenyl ester, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of diposphine rhodium complex for hydrhydroformylation of)
- IT 159398-08-0P 159398-09-1P 159398-10-4P 159516-56-0P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of phosphine compds. and their transition metal complexes)
- IT 108-48-5, 2,6-Lutidine 4559-70-0, Diphenylphosphine oxide 5382-00-3, Chlorodiphenoxyphosphine 6737-42-4, 1,3-Bis(diphenylphosphino)propane 7719-12-2, Phosphorus trichloride 14874-82-9, (Acetylacetonato)dicarbonylrhodium 18531-94-7, (R)-1,1'-Bi-2-naphthol 18531-99-2, (S)-1,1'-Bi-2-naphthol
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of phosphine compds. and their transition metal complexes)
- IT 126613-06-7P 132532-04-8P 137156-22-0P 149917-85-1P 149917-86-2P 149917-87-3P **149917-88-4P 149917-89-5P** 149952-92-1P 155613-52-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of phosphine compds. and their transition metal complexes)
- IT **149917-88-4P 149917-89-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of phosphine compds. and their transition metal complexes)
- RN 149917-88-4 HCAPLUS
- CN [1,1'-Binaphthalen]-2-ol, 2'-(diphenylphosphino)-, (1R)- (9CI) (CA INDEX NAME)

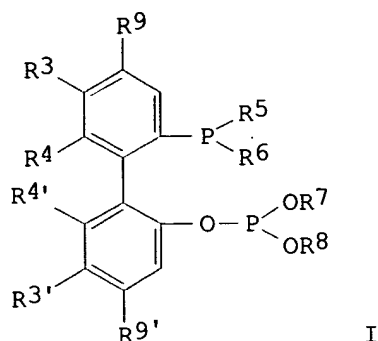


- RN 149917-89-5 HCAPLUS
- CN [1,1'-Binaphthalen]-2-ol, 2'-[bis(3,5-dimethylphenyl)phosphino]-, (R)- (9CI) (CA INDEX NAME)



L81 ANSWER 13 OF 18 HCAPLUS COPYRIGHT 2003 ACS
 AN 1995:231201 HCAPLUS
 DN 122:239952
 TI Preparation of diphosphines and rhodium complexes and their use for
 producing optically active aldehydes and 4-[(R)-1'-formylethyl]azetidin-2-
 one derivatives.
 IN Saito, Takao; Matsumura, Kazuhiko; Kato, Yasushi; Sayo, Noboru;
 Kumobayashi, Hidenori
 PA Takasago International Corporation, Japan
 SO Eur. Pat. Appl., 31 pp.
 CODEN: EPXXDW
 DT **Patent**
 LA English
 IC ICM C07F009-50
 ICS C07F015-00; C07C045-50; C07F009-6574; C07F009-6568; C07D205-08
 CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 26, 67, 78
 FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 614903	A2	19940914	EP 1994-301775	19940311 <--
	EP 614903	A3	19950111		
	EP 614903	B1	20000920		
	R: CH, DE, FR, GB, IT, LI, NL				
	JP 06316560	A2	19941115	JP 1994-54426	19940301 <--
	JP 3277065	B2	20020422		
	JP 2002128759	A2	20020509	JP 2001-328632	19940301 <--
	EP 684249	A1	19951129	EP 1995-111575	19940311 <--
	EP 684249	B1	20030219		
	R: CH, DE, FR, GB, IT, LI, NL				
	EP 684230	A1	19951129	EP 1995-111576	19940311 <--
	EP 684230	B1	20020703		
	R: CH, DE, FR, GB, IT, LI, NL				
PRAI	JP 1993-77484	A	19930312 <--		
	JP 1994-54426	A3	19940301 <--		
	EP 1994-301775	A3	19940311 <--		
OS	CASREACT 122:239952; MARPAT 122:239952				
GI					



- AB The prepn. of novel phosphine compds., e.g. I (R4, R4' = H, lower alkyl, alkoxy; R3, R3', R9, R9' = H, lower alkyl, alkoxy, halo; R3R4, R3'R4' = ring; R5, R6 = (un)substituted Ph, halo, lower alkoxy; R7, R8 = (un)substituted Ph; R7R8 = divalent hydrocarbon), useful in the form of their transition metal complexes, of or compds. with transition metals, in producing an optically active aldehyde by hydroformylation of an olefin with high positional and steric selectivities, are described.
4-[(R)-1'-formylethyl]azetidin-2-one derivs. obtainable by the process is particularly useful as an intermediate for the prepn. of carbapenem antibiotics. Thus, reaction of (+)-3,3'-dichloro-2,2',4,4'-tetramethyl-6-diphenylphosphino-6'-hydroxybiphenyl (prepn. given) with (R)-1,1'-binaphthalene-2,2'-diyldioxychlorophosphine (prepn. given) in PhMe in the presence of Et3N gave (S)-3,3'-dichloro-2,2',4,4'-tetramethyl-6-diphenylphosphinobiphenyl-6'-yloxy((R)-1,1'-binaphthalene-2,2'-diyldioxy)phosphine (II). Hydroformylation of styrene in the presence of Rh(acac)(CO)2 (catalyst) and ligand II gave good yield of (S)-(+)-2-phenylpropanal with 94% enantiomeric excess.
- ST diphosphine ligand prepn catalyst hydroformylation; rhodium diphosphine complex prepn hydroformylation catalyst; aldehyde optically active prepn; azetidinone hydroformylation catalyst; formylethylazetidinone optically active prepn
- IT Stereochemistry
(of hydroformylation of olefins and azetidinones)
- IT Hydroformylation
(of olefins and azetidinones)
- IT Hydroformylation catalysts
(prepn. of diphosphines and rhodium complexes and their use for producing optically active aldehydes and formylethylazetidinone derivs.)
- IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of diphosphines and rhodium complexes and their use for producing optically active aldehydes and formylethylazetidinone derivs.)
- IT Aldehydes, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of diphosphines and rhodium complexes and their use for producing optically active aldehydes and formylethylazetidinone derivs.)
- IT 95-13-6, 1H-Indene 100-42-5, Styrene, reactions 107-01-7, 2-Butene 108-05-4, Vinyl acetate, reactions 447-53-0 592-41-6, 1-Hexene, reactions 112256-72-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroformylation; prepn. of diphosphines and rhodium complexes and their use for producing optically active aldehydes and formylethylazetidinone derivs.)
- IT 3375-31-3, Palladium acetate 12092-47-6 149952-93-2 159398-11-5

159496-99-8

RL: CAT (Catalyst use); USES (Uses)

(prepn. of diphosphines and rhodium complexes and their use for producing optically active aldehydes and formylethylazetidinone derivs.)

IT 31096-69-2

RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

(prepn. of diphosphines and rhodium complexes and their use for producing optically active aldehydes and formylethylazetidinone derivs.)

IT 149917-85-1P 149917-86-2P 149917-87-3P 149952-92-1P 155566-52-2P
155566-53-3P 155613-50-6P 155613-51-7P 159496-88-5P 159496-92-1P
159496-94-3P 159496-96-5P 159573-28-1P 159573-29-2P 159573-30-5P
159573-31-6P 159573-32-7P 159573-33-8P 159573-34-9P

RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of diphosphines and rhodium complexes and their use for producing optically active aldehydes and formylethylazetidinone derivs.)

IT 159398-04-6P 159398-05-7P 159398-06-8P 159398-07-9P 159398-08-0P
159398-09-1P 159398-10-4P 159516-49-1P 159516-56-0P 159518-56-6P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. of diphosphines and rhodium complexes and their use for producing optically active aldehydes and formylethylazetidinone derivs.)

IT 88-04-0, 4-Chloro-3,5-xyleneol 527-54-8, 3,4,5-Trimethylphenol
4559-70-0, Diphenylphosphine oxide 7719-12-2, Phosphorus trichloride
18531-94-7, (R)-1,1'-Bi-2-naphthol 18531-99-2, (S)-1,1'-Bi-2-naphthol
65355-00-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of diphosphines and rhodium complexes and their use for producing optically active aldehydes and formylethylazetidinone derivs.)

IT 17763-95-0P 65355-14-8P 126613-06-7P 132532-04-8P 137156-22-0P
149917-88-4P 155566-49-7P 155566-51-1P 155613-52-8P
159496-80-7P 159496-81-8P 159496-82-9P 159496-83-0P 159496-84-1P
159496-85-2P 159496-86-3P 159496-87-4P 159496-89-6P 159496-90-9P
159496-91-0P 159496-93-2P 159496-95-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of diphosphines and rhodium complexes and their use for producing optically active aldehydes and formylethylazetidinone derivs.)

IT 33204-48-7P 33530-47-1P 38235-74-4P 66875-69-2P 66875-70-5P
66875-71-6P 155566-54-4P 159496-97-6P 159496-98-7P 159573-35-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of diphosphines and rhodium complexes and their use for producing optically active aldehydes and formylethylazetidinone derivs.)

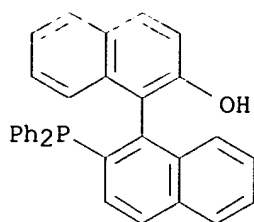
IT 149917-88-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of diphosphines and rhodium complexes and their use for producing optically active aldehydes and formylethylazetidinone derivs.)

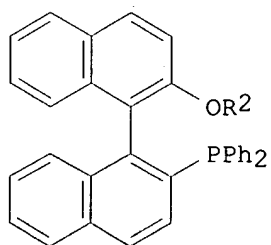
RN 149917-88-4 HCAPLUS

CN [1,1'-Binaphthalen]-2-ol, 2'-(diphenylphosphino)-, (1R)- (9CI) (CA INDEX NAME)



L81 ANSWER 14 OF 18 HCAPLUS COPYRIGHT 2003 ACS
 AN 1995:128170 HCAPLUS
 DN 122:81619
 TI Preparation of optically active trichlorosilanes
 IN Hayashi, Tamio; Uozumi, Yasuhiro; Tanahashi, Asako
 PA Takasago Perfumery Co Ltd, Japan
 SO Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DT **Patent**
 LA Japanese
 IC ICM C07F007-12
 ICS B01J027-18; C07B053-00
 ICA C07B061-00
 CC 29-6 (Organometallic and Organometalloidal Compounds)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06199875	A2	19940719	JP 1991-292676	19911004 <--
	JP 2908919	B2	19990623		
PRAI	JP 1991-292676		19911004	<--	
OS	CASREACT 122:81619; MARPAT 122:81619				
GI					



I

AB Optically active MeCR1SiCl3 (I; R1 = C2-10 alkyl) are prepd. by asym. hydrosilylation of CH2:CHR1 (II; R1 = same as I) by HSiCl3 in presence of optically active phosphines III [R2 = H, C5-7 cycloalkyl, (halo-, lower alkoxy-, or Ph-substituted) C1-6 alkyl] and Pd complexes. A mixt. of 1-octene, HSiCl3, [(π -allyl)PdCl]2, and (S)-(-)-III (R2 = Me) was stirred at 40.degree. for 72 h to give 83% optically active 2-trichlorosilyloctane.

ST chlorosilane optically active prepn; silane trichloro optically active prepn; alkene asym hydrosilylation trichlorosilane catalyst; phosphine alkene asym hydrosilylation trichlorosilane; palladium alkene asym hydrosilylation trichlorosilane

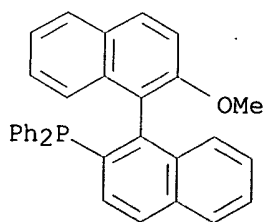
IT Stereochemistry
 (prepn. of optically active trichlorosilanes by asym. hydrosilylation of trichlorosilane to alkenes with phosphines and Pd complexes)

IT Hydrosilylation

Hydrosilylation catalysts

(stereoselective, prepn. of optically active trichlorosilanes by asym. hydrosilylation of trichlorosilane to alkenes with phosphines and Pd complexes)

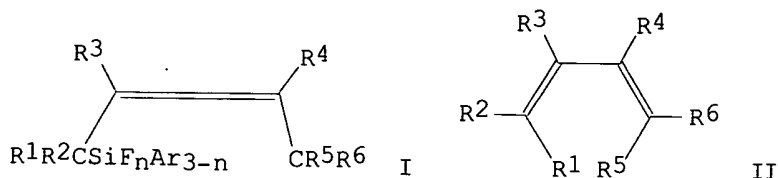
- IT 12012-95-2
RL: CAT (Catalyst use); USES (Uses)
(catalyst; prepn. of optically active trichlorosilanes by asym. hydrosilylation of trichlorosilane to alkenes with phosphines and Pd complexes)
- IT 134484-36-9P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(catalyst; prepn. of optically active trichlorosilanes by asym. hydrosilylation of trichlorosilane to alkenes with phosphines and Pd complexes)
- IT 18225-07-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(optically active; prepn. of optically active trichlorosilanes by asym. hydrosilylation of trichlorosilane to alkenes with phosphines and Pd complexes)
- IT 4559-70-0, Diphenylphosphine oxide 18531-99-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of optically active phosphine catalyst from binaphthol)
- IT 128544-05-8P 134484-37-0P 137769-33-6P 137769-34-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of optically active phosphine catalyst from binaphthol)
- IT 111-66-0, 1-Octene 10025-78-2, Trichlorosilane
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of optically active trichlorosilanes by asym. hydrosilylation of trichlorosilane to alkenes with phosphines and Pd complexes)
- IT 134484-36-9P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(catalyst; prepn. of optically active trichlorosilanes by asym. hydrosilylation of trichlorosilane to alkenes with phosphines and Pd complexes)
- RN 134484-36-9 HCAPLUS
- CN Phosphine, [(1S)-2'-methoxy[1,1'-binaphthalen]-2-yl]diphenyl- (9CI) (CA INDEX NAME)



L81 ANSWER 15 OF 18 HCAPLUS COPYRIGHT 2003 ACS
AN 1994:218162 HCAPLUS
DN 120:218162
TI Optically active allylfluorosilanes and their preparation
IN Hyama, Tamejiro; Hatanaka, Yasuo
PA Sagami Chem Res, Japan
SO Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DT Patent
LA Japanese

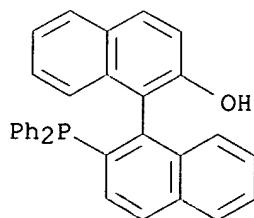
IC ICM C07F007-12
 ICS B01J031-22; B01J031-24
 ICA C07B061-00
 CC 29-6 (Organometallic and Organometalloidal Compounds)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05255353	A2	19931005	JP 1992-88376	19920313 <--
PRAI	JP 1992-88376		19920313 <--		
OS	CASREACT 120:218162; MARPAT 120:218162				
GI					



- AB The title compds. I (R1 - R6 = H, alkyl, aryl, silyl; R1 = R2 .noteq. H; Ar = aryl; R1R2, R2R3, R3R4, R4R5, R5R6, R1R6 may be bonded to form a ring; n = 1, 2, 3), useful as intermediates for optically active allyl alcs., are prepd. by treating butadienes II with HSiFnAr3-n in the presence of group 10 transition metal complex catalysts with optically active ligands. (E)-PhCH:CHCH:CH2 was treated with HSiPhF2 in the presence of PdCl2L [L = (R)-N,N-dimethyl-1-(S)-2-(diphenylphosphinoferrocenyl)ethylamine] at room temp. for 22 h to give 53% (S)-(Z)-PhCH(SiF2Ph)CH:CHMe of 99% e.e.
- ST allylfluorosilane chiral prepn; fluoroallylsilane optically active prepn; hydrosilane reaction butadiene; hydrosilylation asym butadiene; group 10 catalyst hydrosilylation butadiene; allyl alc chiral intermediate allylsilane
- IT Asymmetric synthesis and induction
 (of allylfluorosilanes, by group 10 metal-catalyzed hydrosilylation of butadienes)
- IT Alcohols, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (allyl, prepn. of, optically active fluoroallylsilanes as intermediates for)
- IT Group VIII element compounds
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (complexes, chiral, catalysts, for asym. hydrosilylation of butadienes)
- IT Silanes
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (fluoro, allyl, chiral, prepn. of, by asym. hydrosilylation of butadienes, catalysts for)
- IT Hydrosilylation catalysts
 (stereoselective, chiral group 10 metal complexes, for butadienes with fluorohydrosilanes)
- IT 71307-87-4 76374-09-9
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst, for asym. hydrosilylation of butadienes with fluorohydrosilanes)
- IT 12012-95-2, Allylchloropalladium dimer 149917-88-4
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts contg., for asym. hydrosilylation of butadienes with fluorohydrosilanes)
- IT 1631-83-0, Chlorodiphenylsilane 1631-84-1, Dichlorophenylsilane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (fluorination of)

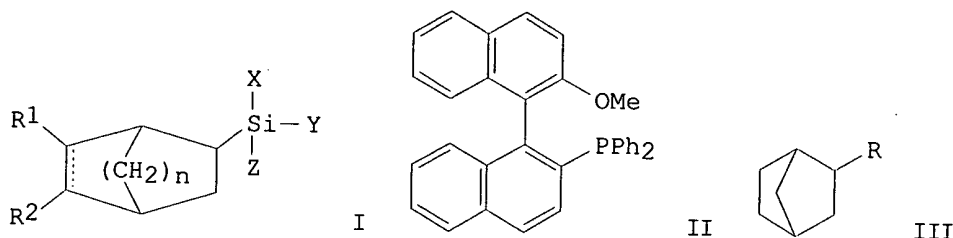
- IT 542-92-7, Cyclopentadiene, uses 2004-70-8, (E)-1,3-Pentadiene
16939-57-4, (E)-1-Phenyl-1,3-butadiene
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrosilylation of, by fluorohydrosilanes, stereoselective, chiral
group 10 metal complex catalysts for)
- IT 696-35-5P, Difluorophenylsilane 1013-91-8P, Fluorodiphenylsilane
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and asym. hydrosilylation by, of butadienes, chiral group 10
metal catalysts for)
- IT 22135-49-5P, (S)-1-Phenyl-1-butanol 22144-60-1P, (R)-1-Phenyl-1-butanol
102339-78-6P, (R)-2-Pentyl benzoate 153841-08-8P, (S)-(Z)-1-Phenyl-1-
triphenylsilyl-2-butene 153841-09-9P, (R)-(Z)-4-(Triphenylsilyl)-2-
pentene
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 64770-02-1P, 3-(Methyldiphenylsilyl)cyclopentene
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of optically active)
- IT 153841-05-5P, 3-(Fluorodiphenylsilyl)cyclopentene
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of optically active, as intermediates for allyl alcs.)
- IT 153841-03-3P 153841-04-4P, (R)-(Z)-4-(Difluorophenylsilyl)-2-pentene
153841-06-6P 153841-07-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for chiral allyl alcs.)
- IT 153841-02-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, catalysts contg., for asym. hydrosilylation of butadienes
with fluorohydrosilanes)
- IT 115793-56-1P, (S)-(Z)-1-Phenyl-2-buten-1-ol
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, optically active allylfluorosilanes as intermediates for)
- IT 18162-48-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(silylation by, of hydroxydiphenylphosphinobinaphthyl)
- IT 149917-88-4
RL: CAT (Catalyst use); USES (Uses)
(catalysts contg., for asym. hydrosilylation of butadienes with
fluorohydrosilanes)
- RN 149917-88-4 HCAPLUS
- CN [1,1'-Binaphthalen]-2-ol, 2'-(diphenylphosphino)-, (1R)- (9CI) (CA INDEX
NAME)



L81 ANSWER 16 OF 18 HCAPLUS COPYRIGHT 2003 ACS
AN 1994:218160 HCAPLUS
DN 120:218160
TI Preparation of optically active silylbicycloalkane or -alkene compounds
IN Hayashi, Tamio; Uozumi, Yasuhiro
PA Kanegafuchi Chemical Ind, Japan
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF

DT Patent
 LA Japanese
 IC ICM C07F007-08
 ICS C07F007-10; C07F007-14; C07F007-18
 CC 29-6 (Organometallic and Organometalloidal Compounds)
 FAN.CNT 1

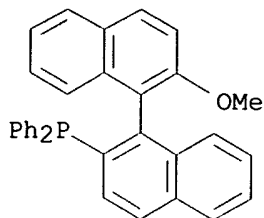
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05255351	A2	19931005	JP 1992-51389	19920310 <--
	JP 3279620	B2	20020430		
PRAI	JP 1992-51389		19920310 <--		
OS	MARPAT 120:218160				
GI					



AB The title compds. [I; R₁, R₂ = H, alkyl, aralkyl, aryl, alkoxy, carbonyl, cyano, NO₂; X, Y, Z = H, alkyl, alkoxy, halo; n = 1, 2; dotted line = unsatd. or satd.] are prepd. by asym. hydrosilylation of unsatd. bicyclic compds. in the presence of chiral phosphine catalysts. A mixt. of norbornene, HSiCl₃, allylpalladium chloride dimer, and (R)-(+)-II was stirred under cooling, then heated at 100.degree. to give 95.5% (1S, 2S, 4R)-II (R = SiCl₃), which was treated with EtOH and Et₃N in Et₂O at room temp. to give 86% (1S, 2S, 4R)-III [R = Si(OEt)₃]. Hydroxylation of the silyl ether with KHCO₃ and H₂O₂ in MeOH/THF at 50.degree. gave 72% exo-norborneol.

ST chiral silylbicycloalkane; asym hydrosilylation norbornene bicyclooctene
 IT Hydrosilylation
 (asym., of norbornene and bicyclooctene derivs.)
 IT 121-46-0, Norbornadiene 498-66-8, Norbornene 931-64-6,
 Bicyclo[2.2.2]octene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (asym. hydrosilylation of, chiral catalysts for)
 IT 145964-33-6
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst, for asym. hydrosilylation of norbornene)
 IT 146075-48-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and ethoxylation of)
 IT 153924-15-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and hydrolysis of)
 IT 280-33-1P, Bicyclo[2.2.2]octane 497-37-0P 2890-98-4P,
 exo-5-Hydroxy-2-norbornene 65118-94-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 IT 145964-33-6
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst, for asym. hydrosilylation of norbornene)
 RN 145964-33-6 HCAPLUS
 CN Phosphine, [(1R)-2'-methoxy[1,1'-binaphthalen]-2-yl]diphenyl- (9CI) (CA

INDEX NAME)



L81 ANSWER 17 OF 18 HCAPLUS COPYRIGHT 2003 ACS

AN 1994:133865 HCAPLUS

DN 120:133865

TI Preparation of optically active 1-alkenes as intermediates for terpenes

IN Hayashi, Tamio; Matsumoto, Yonetatsu; Naito, Masaki

PA Kuraray Co, Japan

SO Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DT **Patent**

LA Japanese

IC ICM C07C011-12

ICS B01J031-04; B01J031-24; C07C001-213; C07C001-30; C07C011-02

ICA C07B061-00

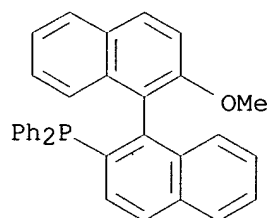
CC 23-17 (Aliphatic Compounds)

Section cross-reference(s): 30

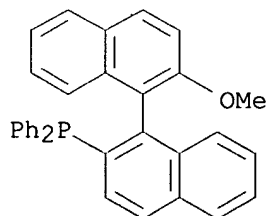
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	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05238964	A2	19930917	JP 1992-76311	19920227 <--
	JP 3120409	B2	20001225		
PRAI	JP 1992-76311		19920227 <--		
OS	CASREACT 120:133865; MARPAT 120:133865				
AB	R1R2CHCH:CH2 [R1, R2 = (un)substituted alkyl, (un)substituted alkenyl, (un)substituted aryl; R1 .noteq. R2] are prepd. by asym. redn. of R1R2C:CHCH2X (R1, R2 = same as above; X = leaving group) in the presence of Pd compds., optically active phosphines, tertiary amines, and HCO2H. Geranyl acetate was treated with tris(dibenzylideneacetone)dipalladium-chloroform, (S)-2-diphenylphosphino-2'-methoxy-1,1'-binaphthyl, Et3N, and HCO2H in THF at 40.degree. for 4 h to give 94% (R)-3,7-dimethyl-1,6-octadiene (55% ee).				
ST	optically active alkene intermediate terpene; asym redn unsatd acetate; palladium phosphine additive asym redn; tertiary amine formate asym redn				
IT	Terpenes and Terpenoids, preparation				
	RL: PREP (Preparation)				
	(intermediates for, optically active alkenes as)				
IT	Reduction				
	(stereoselective, of unsatd. acetates, in prepn. of optically active alkenes as intermediates for terpenes)				
IT	Amines, uses				
	RL: USES (Uses)				
	(tertiary, in asym. redn. of unsatd. acetates)				
IT	Alkenes, preparation				
	RL: SPN (Synthetic preparation); PREP (Preparation)				
	(.alpha.-, prepn. of, optically active, as intermediates for terpenes)				
IT	62-53-3, Aniline, reactions				
	RL: RCT (Reactant); RACT (Reactant or reagent)				
	(amidation of, with dicarboxylic acid)				
IT	105-87-3, Geranyl acetate 141-12-8, Neryl acetate				
	RL: RCT (Reactant); RACT (Reactant or reagent)				

- (asym. redn. of)
- IT 64-18-6, Formic acid, uses 121-44-8, Triethylamine, uses
RL: USES (Uses)
(in asym. redn. of unsatd. acetates)
- IT 51364-51-3, Tris(dibenzylideneacetone)dipalladium 134484-36-9,
(S)-(-)-2-Diphenylphosphino-2'-methoxy-1,1'-binaphthyl 145964-33-6
, (R)-(+)-2-Diphenylphosphino-2'-methoxy-1,1'-binaphthyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(in asym. redn. of unsatd. acetates)
- IT 1115-82-8P 153279-32-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
- IT 10281-55-7P, (S)-3,7-Dimethyl-1,6-octadiene 10281-56-8P,
(R)-3,7-Dimethyl-1,6-octadiene
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, from unsatd. acetate, as intermediate for terpenes)
- IT 134484-36-9, (S)-(-)-2-Diphenylphosphino-2'-methoxy-1,1'-
binaphthyl 145964-33-6, (R)-(+)-2-Diphenylphosphino-2'-methoxy-
1,1'-binaphthyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(in asym. redn. of unsatd. acetates)
- RN 134484-36-9 HCAPLUS
- CN Phosphine, [(1S)-2'-methoxy[1,1'-binaphthalen]-2-yl]diphenyl- (9CI) (CA
INDEX NAME)



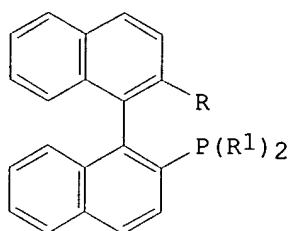
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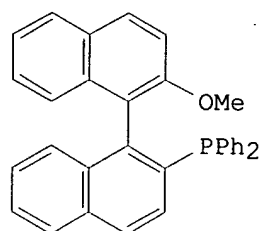
- L81 ANSWER 18 OF 18 HCAPLUS COPYRIGHT 2003 ACS
- AN 1993:7190 HCAPLUS
- DN 118:7190
- TI Preparation of optically active binaphthylphosphines as components of
enantioselective hydrosilylation catalysts
- IN Hayashi, Tamio; Uozumi, Yasuhiro; Yamazaki, Akiko; Kumobayashi, Hidenori
- PA Takasago International Corp., Japan
- SO Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
- DT Patent
- LA English

IC ICM C07F009-50
ICS C07F015-00; B01J031-28
CC 29-7 (Organometallic and Organometalloidal Compounds)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	EP 503884	B1	19950726		
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	JP 05017491	A2	19930126	JP 1991-266864	19910919 <--
	JP 2733880	B2	19980330		
	US 5231202	A	19930727	US 1992-850998	19920312 <--
PRAI	JP 1991-70339		19910312		<--
	JP 1991-266864		19910919		<--
OS	MARPAT 118:7190				
GI					



I



II

- AB Title compds. [I; R = alkyl, OR₂; R₁ = Ph, pentafluorophenyl; R₂ = H, cycloalkyl, (halo)alkyl, (alkoxy)alkoxy, Ph), were prepd. Thus, (S)-2,2'-binaphthol was stirred with (F₃CSO₂)₂ and pyridine in CH₂Cl₂ overnight to give 92% bis-triflate which was stirred with Ph₂P(O)H, Pd(OAc)₂, and 1,4-bis(diphenylphosphino)butane in Me₂SO at 100.degree. for 12 h to give 96% (S)-(-)-2-trifluoromethanesulfonyl-2'-diphenylphosphinoyl-1,1'-binaphthyl. The latter was hydrolyzed with 3N NaOH in MeOH/dioxane in 81.5% yield and the product was O-methylated with MeI/K₂CCO₃/acetone (98%) and reduced with Cl₃SiH/Et₃N in xylene (79%) to give 19% (S)-II. This was used to enantioselectively hydrosilylate 1-phenyl-1,3-butadiene with Cl₃SiH.
- ST binaphthylphosphine alkoxy prepn hydrosilylation catalyst
- IT Hydrosilylation catalysts
(binaphthylphosphines)
- IT Hydrosilylation
(by trichlorosilane)
- IT 925-90-6, Ethylmagnesium bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with triflyloxydiphenylphosphinoylbinaphthyl)
- IT 75-30-9, Isopropyl iodide
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of hydroxydiphenylphosphinoylbinaphthyl)
- IT 100-39-0, Benzylbromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylation by, of hydroxydiphenylphosphinoylbinaphthyl)
- IT 18531-99-2
RL: PROC (Process)
(conversion of, to triflate diester, in prepn. of enantioselective hydrosilylation catalyst)
- IT 1515-78-2, 1-Phenyl-1,3-butadiene
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective hydrosilylation of, naphthylphosphine catalysts for)
- IT 10025-78-2, Trichlorosilane
RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrosilylation by, of phenylbutadiene, enantioselective by naphthylphosphinehydrosilylation catalysts for)

IT 3347-57-7P 81176-43-4P 144868-13-3P 144868-14-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 134484-36-9P 137769-31-4P 144868-17-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as enantioselective hydrosilylation catalyst)

IT 137769-30-3P 144868-15-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as in enantioselective hydrosilylation catalyst)

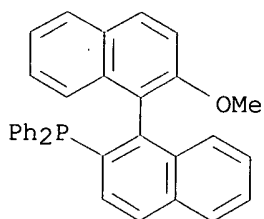
IT 137769-28-9P 144868-16-6P
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IT 128544-05-8P 134484-37-0P 137769-27-8P 137769-33-6P 137769-34-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
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IT 134484-36-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as enantioselective hydrosilylation catalyst)

RN 134484-36-9 HCAPLUS

CN Phosphine, [(1S)-2'-methoxy[1,1'-binaphthalen]-2-yl]diphenyl- (9CI) (CA INDEX NAME)



=> fil reg

FILE 'REGISTRY' ENTERED AT 10:00:04 ON 12 MAY 2003

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STRUCTURE FILE UPDATES: 11 MAY 2003 HIGHEST RN 514167-89-6

DICTIONARY FILE UPDATES: 11 MAY 2003 HIGHEST RN 514167-89-6

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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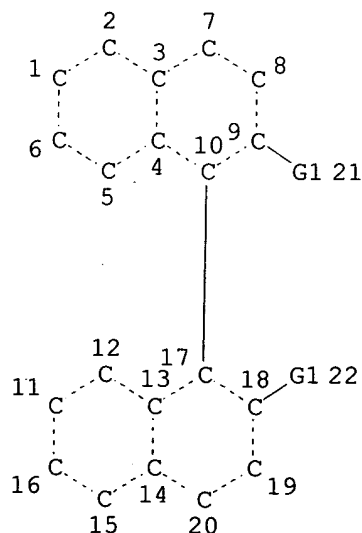
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L19

STR



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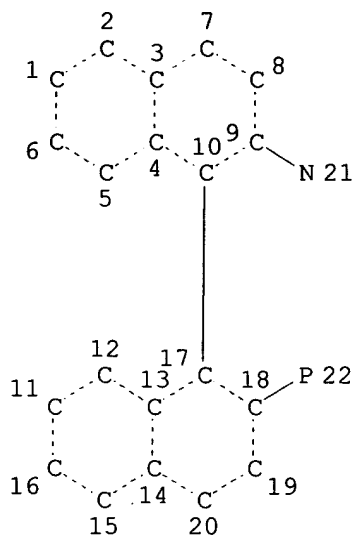
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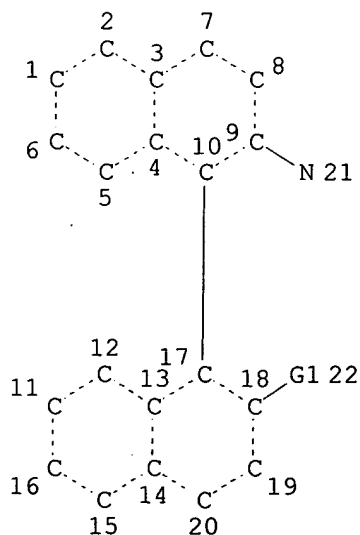
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NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

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L53 STR



VAR G1=AS/O/S

NODE ATTRIBUTES:

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

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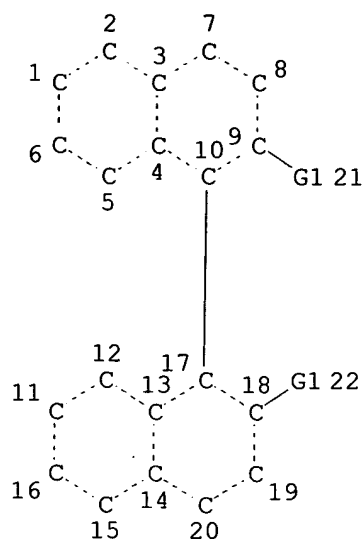
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169 ANSWERS

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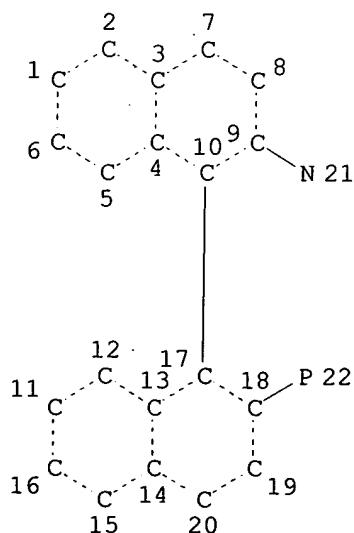
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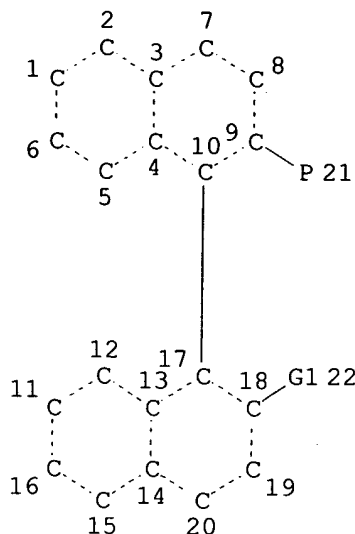
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257 ANSWERS

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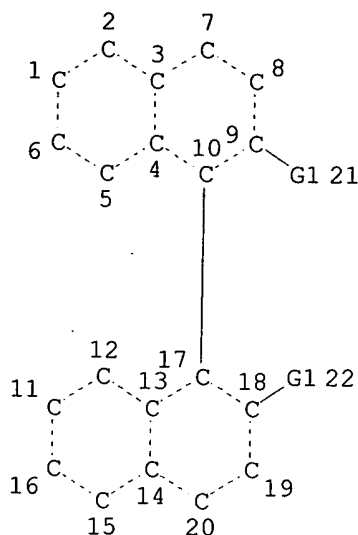
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GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

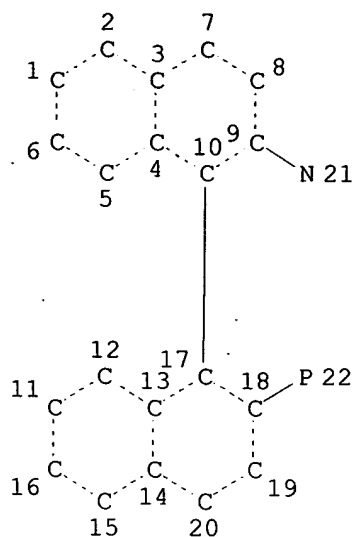
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L21 6721 SEA FILE=REGISTRY SSS FUL L19

L22 6718 SEA FILE=REGISTRY ABB=ON PLU=ON L21 NOT L11

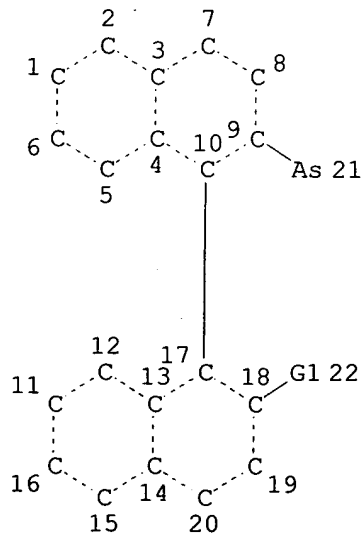
L46 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE
 L48 75 SEA FILE=REGISTRY SUB=L22 SSS FUL L46
 L54 6643 SEA FILE=REGISTRY ABB=ON PLU=ON L22 NOT L48
 L59 STR



VAR G1=O/S
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L60 0 SEA FILE=REGISTRY SUB=L54 SSS FUL L59

100.0% PROCESSED 0 ITERATIONS

0 ANSWERS

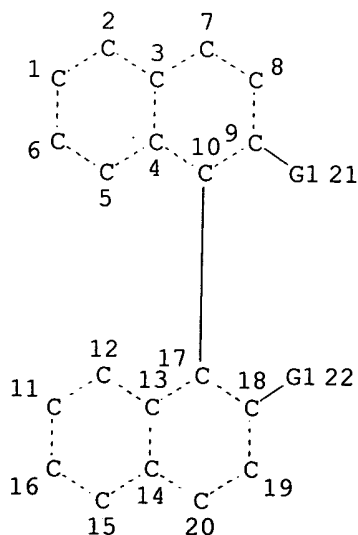
SEARCH TIME: 00.00.01

=> d sta que 162

L10 486 SEA FILE=REGISTRY ABB=ON PLU=ON (100-00-5/BI OR 100-46-9/BI
 OR 100-61-8/BI OR 1003-09-4/BI OR 1013-88-3/BI OR 10282-31-2/BI
 OR 103-88-8/BI OR 106-38-7/BI OR 106-41-2/BI OR 106-43-4/BI
 OR 106-49-0/BI OR 1079-66-9/BI OR 108-94-1/BI OR 110-91-8/BI
 OR 111-26-2/BI OR 111-92-2/BI OR 1122-91-4/BI OR 1126-46-1/BI
 OR 120-72-9/BI OR 123-75-1/BI OR 128796-39-4/BI OR 13716-10-4/B
 I OR 138900-16-0/BI OR 14221-01-3/BI OR 157282-19-4/BI OR
 16523-54-9/BI OR 167283-32-1/BI OR 17057-88-4/BI OR 171092-38-9
 /BI OR 174307-96-1/BI OR 17933-03-8/BI OR 180336-54-3/BI OR
 18982-54-2/BI OR 197172-67-1/BI OR 19853-10-2/BI OR 204841-19-0
 /BI OR 2052-07-5/BI OR 20837-12-1/BI OR 213697-51-9/BI OR
 213697-52-0/BI OR 213697-53-1/BI OR 213697-65-5/BI OR 213697-66
 -6/BI OR 213697-67-7/BI OR 213774-71-1/BI OR 2142-66-7/BI OR
 2142-68-9/BI OR 22237-13-4/BI OR 224311-51-7/BI OR 224311-54-0/
 BI OR 224311-55-1/BI OR 224311-57-3/BI OR 224311-58-4/BI OR
 224311-59-5/BI OR 23676-05-3/BI OR 251320-77-1/BI OR 251320-78-
 2/BI OR 251320-81-7/BI OR 251320-82-8/BI OR 251320-84-0/BI OR
 251320-89-5/BI OR 255835-81-5/BI OR 255835-82-6/BI OR 255835-83
 -7/BI OR 255835-84-8/BI OR 255835-85-9/BI OR 255837-14-0/BI OR
 255837-15-1/BI OR 255837-16-2/BI OR 255882-14-5/BI OR 2856-63-5
 /BI OR 2920-38-9/BI OR 2928-43-0/BI OR 31144-33-9/BI OR
 3375-31-3/BI OR 39253-43-5/BI OR 3972-65-4/BI OR 3976-34-9/BI
 OR 39910-98-0/BI OR 40138-16-7/BI OR 402-43-7/BI OR 4075-79-0/B
 I OR 42371-64-2/BI OR 460-00-4/BI OR 4688-76-0/BI OR 51364-51-3
 /BI OR 534-17-8/BI OR 53847-33-9/BI OR 54000-83-8/BI OR
 5405-15-2/BI OR 54660-04-7/BI OR 553-94-6/BI OR 556-96-7/BI OR
 563-80-4/BI OR 565-69-5/BI OR 5720-06-9/BI OR 576-22-7/BI OR
 583-53-9/BI OR 583-55-1/BI OR 592-41-6/BI OR 59734-92-8/BI OR
 613-37-6/BI OR 619-42-1/BI OR 623-03-0/BI OR 623-12-1/BI OR
 626-60-8/BI OR 644-08-6/BI OR 6476-37-5

L11

3 SEA FILE=REGISTRY ABB=ON PLU=ON L10 AND C34H40NP
 L19 STR



VAR G1=N/P/AS/O/S

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

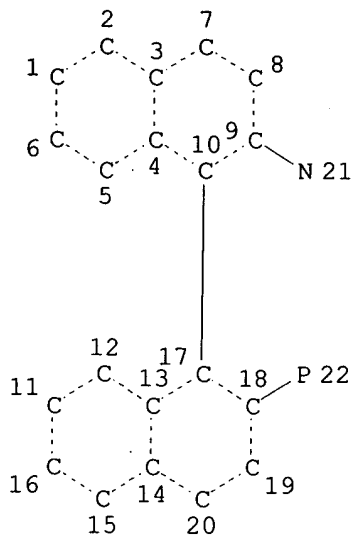
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L21 6721 SEA FILE=REGISTRY SSS FUL L19

L22 6718 SEA FILE=REGISTRY ABB=ON PLU=ON L21 NOT L11

L46 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

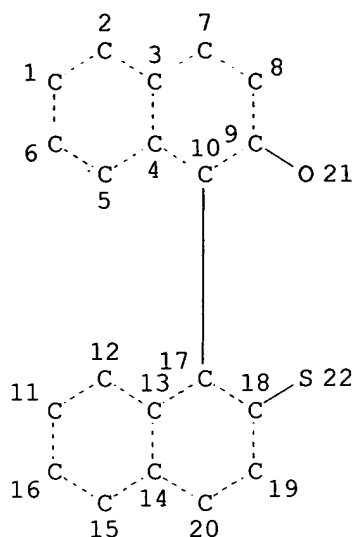
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L48 75 SEA FILE=REGISTRY SUB=L22 SSS FUL L46

L54 6643 SEA FILE=REGISTRY ABB=ON PLU=ON L22 NOT L48

L61 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE
 L62 56 SEA FILE=REGISTRY SUB=L54 SSS FUL L61

100.0% PROCESSED 276 ITERATIONS
 SEARCH TIME: 00.00.01

56 ANSWERS

=> d his

(FILE 'HOME' ENTERED AT 08:44:27 ON 12 MAY 2003)
 SET COST OFF

FILE 'HCAPLUS' ENTERED AT 08:44:46 ON 12 MAY 2003

	E BUCHWALD S/AU
L1	296 S E3,E4,E6-E9
	E OLD D/AU
L2	15 S E3,E5,E7,E8
	E WOLFE J/AU
L3	201 S E3,E17,E18
	E WOLFE JOHN/AU
L4	38 S E3,E11,E12
	E PALUCKI M/AU
L5	26 S E3,E4
	E KAMIKAWA K/AU
L6	22 S E3,E8
L7	5 S E9-E12
L8	2 S (US20020156295 OR US6307087 OR US6395916)/PN OR WO99-US15450/
L9	2 S L1-L7 AND L8
	SEL RN

FILE 'REGISTRY' ENTERED AT 08:47:36 ON 12 MAY 2003

L10 486 S E1-E486

L11 3 S L10 AND C34H40NP
SEL RN
L12 0 S E487-E489/CRN

FILE 'HCAOLD' ENTERED AT 08:50:52 ON 12 MAY 2003
L13 0 S L11

FILE 'HCAPLUS' ENTERED AT 08:50:58 ON 12 MAY 2003
L14 7 S L11
L15 6 S L14 AND L1-L9
L16 1 S L14 NOT L15
L17 7 S L15,L16

FILE 'USPATFULL, USPAT2' ENTERED AT 08:51:23 ON 12 MAY 2003
L18 3 S L11

FILE 'REGISTRY' ENTERED AT 08:52:42 ON 12 MAY 2003

FILE 'USPATFULL, USPAT2' ENTERED AT 08:52:53 ON 12 MAY 2003

FILE 'HCAPLUS' ENTERED AT 08:53:44 ON 12 MAY 2003

FILE 'REGISTRY' ENTERED AT 08:54:49 ON 12 MAY 2003
L19 STR
L20 50 S L19
L21 6721 S L19 FUL
SAV TEMP L21 SACKKEY004/A
L22 6718 S L21 NOT L11
L23 7 S L22 AND L10
L24 5728 S L22 NOT (PMS OR CCS OR MNS)/CI

FILE 'HCAPLUS' ENTERED AT 08:59:36 ON 12 MAY 2003
L25 4102 S L22
L26 44 S L1-L9 AND L25
SEL HIT RN

FILE 'REGISTRY' ENTERED AT 09:00:08 ON 12 MAY 2003
L27 50 S E490-E539

FILE 'HCAPLUS' ENTERED AT 09:01:02 ON 12 MAY 2003
L28 2247 S L27
L29 44 S L26 AND L28
L30 22 S L29 AND (PY<=1998 OR PRY<=1998 OR AY<=1998)
L31 7 S L30 AND ORGANOMETAL?/SC,SX
L32 35 S L27 (L) CAT/RL AND L29
L33 15 S L30 AND L32
L34 19 S L31,L33

FILE 'REGISTRY' ENTERED AT 09:03:53 ON 12 MAY 2003

FILE 'HCAPLUS' ENTERED AT 09:04:07 ON 12 MAY 2003
L35 3 S L30 NOT L34
L36 3933 S L24,L28 NOT L17,L26,L29-L35
L37 2375 S L36 AND (PY<=1998 OR PRY<=1998 OR AY<=1998)
L38 365 S L37 AND ORGANOMETAL?/SC,SX
L39 1358 S L25(L)CAT/RL
L40 895 S L28(L)CAT/RL
L41 578 S L37 AND L39,L40
L42 116 S L38 AND L41
L43 516 S L37 AND LIGAND
L44 69 S L43 AND L42
SEL HIT RN

FILE 'REGISTRY' ENTERED AT 09:36:26 ON 12 MAY 2003

L45 230 S E540-E770
L46 STR L19
L47 2 S L46 SAM SUB=L22
L48 75 S L46 FUL SUB=L22
SAV L48 SACKY004A/A

FILE 'HCAPLUS' ENTERED AT 09:39:41 ON 12 MAY 2003

L49 30 S L48
L50 7 S L49 AND (PY<=1998 OR PRY<=1998 OR AY<=1998)
L51 5 S L50 NOT L29-L34
L52 2 S L51 AND (PD<=19980710 OR PRD<=19980710 OR AD<=19980710)

FILE 'REGISTRY' ENTERED AT 09:41:46 ON 12 MAY 2003

FILE 'HCAPLUS' ENTERED AT 09:41:53 ON 12 MAY 2003

FILE 'REGISTRY' ENTERED AT 09:42:30 ON 12 MAY 2003

L53 STR L19
L54 6643 S L22 NOT L48
L55 3 S L53 SAM SUB=L54
L56 169 S L53 FUL SUB=L54
SAV L56 SACKY044B/A
L57 STR L53
L58 257 S L57 FUL SUB=L54
DEL SACKY044B/A
SAV L56 SACKY004B/A
SAV L58 SACKY004C/A
L59 STR L57
L60 0 S L59 FUL SUB=L54
SAV L60 SACKY004D/A
L61 STR L59
L62 56 S L61 FUL SUB=L54
SAV L62 SACKY004E/A

FILE 'HCAPLUS' ENTERED AT 09:46:41 ON 12 MAY 2003

L63 243 S L56 OR L58 OR L62
L64 138 S L63 AND (PD<=19980710 OR PRD<=19980710 OR AD<=19980710)
L65 70 S L64 AND LIGAND
L66 57 S L64 AND ORGANOMETAL?/SC,SX
L67 146 S L63 (L) CAT/RL
L68 132 S L63 (L) (RACT OR RCT OR RGT)/RL
L69 124 S L64 AND L67,L68
L70 86 S L65,L66 AND L69
L71 63 S L70 NOT P/DT
L72 23 S L70 NOT L71
SEL HIT RN

FILE 'REGISTRY' ENTERED AT 09:49:05 ON 12 MAY 2003

L73 79 S E771-E849
L74 7 S L73 AND (C32H22BROP OR C33H25OP OR C33H23CL2OP OR C36H31OP OR
L75 14 S L73 AND (C33H25O2P OR C32H22BRO2P OR C35H29OP OR C41H29O2P OR
L76 11 S L75 NOT L74
SEL RN 1 4 5 8
L77 4 S E850-E853

FILE 'HCAPLUS' ENTERED AT 09:58:25 ON 12 MAY 2003

L78 93 S L74 OR L77
L79 16 S L78 AND L72
L80 60 S L78 AND (PD<=19980710 OR PRD<=19980710 OR AD<=19980710)
L81 18 S L80 AND P/DT

FILE 'HCAPLUS' ENTERED AT 09:59:44 ON 12 MAY 2003

FILE 'REGISTRY' ENTERED AT 10:00:04 ON 12 MAY 2003